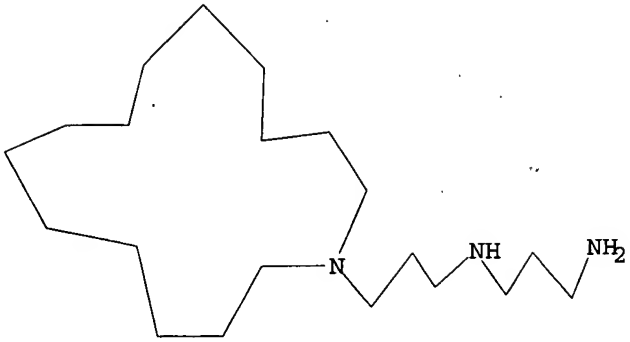

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED -     45 TO ITERATE

100.0% PROCESSED      45 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          498 TO     1302
PROJECTED ANSWERS:               0 TO        0

L2             0 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 09:42:25 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   1026 TO ITERATE

100.0% PROCESSED    1026 ITERATIONS                               1 ANSWERS
SEARCH TIME: 00.00.01

L3             1 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                              148.95     149.16

FILE 'CAPLUS' ENTERED AT 09:42:37 ON 06 AUG 2003
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FILE COVERS 1907 - 6 Aug 2003 VOL 139 ISS 6
FILE LAST UPDATED: 5 Aug 2003 (20030805/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 2 L3

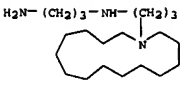
=> d ibib abs hitstr tot

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:574910 CAPLUS
DOCUMENT NUMBER: 137:119652
TITLE: Antiangiogenic compounds and an assay for inhibitors of cell invasion
INVENTOR(S): Roskelley, Calvin; Andersen, Raymond; Williams, David; Roberge, Michel; Dedhar, Shoukat; Karsan, Aly; Minchinton, Andrew
PATENT ASSIGNEE(S): The University of British Columbia, Can.
SOURCE: PCT Int. Appl., 56 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002058679	A2	20020801	WO 2002-CA97	20020125
WO 2002058679	A3	20030515		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003004149	A1	20030102	US 2002-57846	20020125
PRIORITY APPLN. INFO.:			CA 2001-2332138 A	20010125
			US 2001-330670P P	20011026

OTHER SOURCE(S): MARPAT 137:119652
AB This invention provides the use of macrocyclic amines for inhibition of cellular invasion or angiogenesis. Compds. and pharmaceutical compns. of this invention are useful in the treatment of conditions characterized by cellular invasion or angiogenesis, including cancer. Compds. that may be used in this invention include the motuporamines, which are isolated from methanol exts. of Xestospongia exigua.
IT 211569-33-4, Dihydromotuporamine C
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antiangiogenic macrocyclic amines and assays for inhibitors of cell invasion)
RN 211569-33-4 CAPLUS
CN 1,3-Propanediamine, N-[3-(azacyclopentadec-1-yl)propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

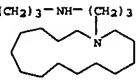


L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:893633 CAPLUS
DOCUMENT NUMBER: 136:164301
TITLE: Motuporamines, anti-invasion and anti-angiogenic, alkaloids from the marine sponge Xestospongia exigua (Kirkpatrick): Isolation, structure elucidation, analogue synthesis, and conformational analysis
AUTHOR(S): Williams, David E.; Craig, Kyle S.; Patrick, Brian; McHardy, Lianne M.; van Soest, Rob; Roberge, Michel; Andersen, Raymond J.
CORPORATE SOURCE: Departments of Chemistry Oceanography (EOS) Biochemistry and Molecular Biology, University of British Columbia, Vancouver, BC, Can.
SOURCE: Journal of Organic Chemistry (2002), 67(1), 245-258
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Exts. of the sponge Xestospongia exigua collected in Papua New Guinea were pos. in a new assay for anti-invasion activity. Bioassay-guided fractionation led to the identification of the three known motuporamines A, B, and C along with the new motuporamines D (e.g. I), E, and F and a mixt. of G, H, and I. Motuporamines A, B, and C and the mixt. of G, H, and I were responsible for the anti-invasion activity of the crude ext. Motuporamine C has also been found to be anti-angiogenic. A series of analogs of the motuporamines have been synthesized and evaluated for anti-invasive activity. These SAR results revealed that a satd. 15-membered cyclic amine fused to the natural motuporamine diamine side chain (II) represented the optimal structure for anti-invasive activity in this family. Single-crystal X-ray diffraction anal. of one of the analogs (III) showed that in the solid state its 16-membered macrocyclic amine fragment adopted the [4444] quadrangular conformation predicted by calcns. to be the lowest energy conformation for the corresponding cycloalkane, cyclohexadecane. These data along with literature X-ray data and conformational anal. for derivs. of azacyclotridecane have been used as precedents for predicting the lowest energy ring conformations of other motuporamines. The SAR data from the natural and synthetic motuporamines have been combined with the conformational analyses to provide an outline of the functionality and shape required for activity in this family of alkaloids and to design a new analog (IV) that showed good anti-invasion activity.
IT 211569-33-4P, Dihydromotuporamine C
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and anti-invasive activity of)
RN 211569-33-4 CAPLUS
CN 1,3-Propanediamine, N-[3-(azacyclopentadec-1-yl)propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY    SESSION
FULL ESTIMATED COST                                    9.49     158.65

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                      ENTRY    SESSION
CA SUBSCRIBER PRICE                                   -1.30      -1.30

STN INTERNATIONAL LOGOFF AT 09:43:12 ON 06 AUG 2003
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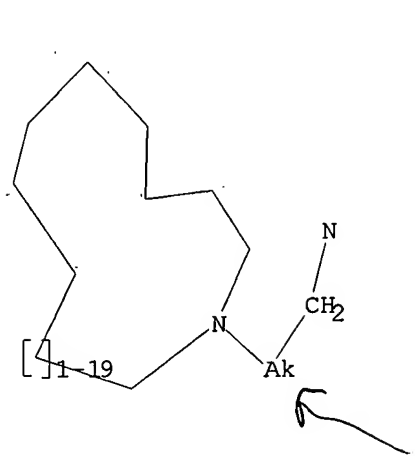

Broad search

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED -  21134 TO ITERATE

  4.7% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       413992 TO   431368
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 10:48:37 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 423315 TO ITERATE

 94.5% PROCESSED  400000 ITERATIONS                             147 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.07

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       423315 TO   423315
PROJECTED ANSWERS:             147 TO      192

L3          147 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             148.15     148.36

FILE 'CAPLUS' ENTERED AT 10:48:51 ON 06 AUG 2003
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FILE COVERS 1907 - 6 Aug 2003 VOL 139 ISS 6
FILE LAST UPDATED: 5 Aug 2003 (20030805/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 28 L3

=> s l4 and angiogenesis?
L5 3 L4 AND ANGIOGENESIS?

=> d ibib abs hitstr tot

L5 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:574910 CAPLUS
DOCUMENT NUMBER: 137:119652
TITLE: Antiangiogenic compounds and an assay for inhibitors of cell invasion
INVENTOR(S): Roskelley, Calvin; Andersen, Raymond; Williams, David; Roberge, Michel; Dedhar, Shoukat; Karsan, Aly; Minchinton, Andrew
PATENT ASSIGNEE(S): The University of British Columbia, Can.
SOURCE: PCT Int. Appl., 56 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002058679	A2	20020801	WO 2002-CA97	20020125
WO 2002058679	A3	20030515		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2003004149	A1	20030102	US 2002-57846		20020125

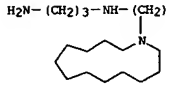
PRIORITY APPLN. INFO.: CA 2001-2332138 A 20010125
US 2001-330670P P 20011026
OTHER SOURCE(S): MARPAT 137:119652

AB This invention provides the use of macrocyclic amines for inhibition of cellular invasion or **angiogenesis**. Compds. and pharmaceutical compns. of this invention are useful in the treatment of conditions characterized by cellular invasion or **angiogenesis**, including cancer. Compds. that may be used in this invention include the motuporamines, which are isolated from methanol exts. of Xestospongia exigua.

IT **398144-70-2**, Motuporamine G **398144-76-8**, Motuporamine H **398144-77-9**, Motuporamine I
RL: NPO (Natural product occurrence); BIOL (Biological study); OCCU (Occurrence)
(antiangiogenic macrocyclic amines and assays for inhibitors of cell invasion)

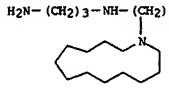
RN 398144-70-2 CAPLUS
CN 1,3-Propanediamine, N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

L5 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



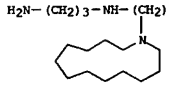
D1-Me

RN 398144-76-8 CAPLUS
CN 1,3-Propanediamine, N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



D1-Me

RN 398144-77-9 CAPLUS
CN 1,3-Propanediamine, N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

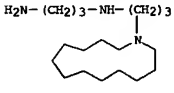


D1-Me

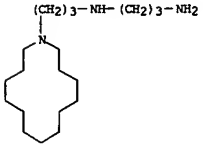
IT **211566-77-7**, Motuporamine A **211566-78-8**, Motuporamine B **211569-34-5**, Motuporamine C **398144-67-7**, Motuporamine D
RL: NPO (Natural product occurrence); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES (Uses)
(antiangiogenic macrocyclic amines and assays for inhibitors of cell invasion)

RN 211566-77-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)

L5 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

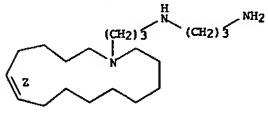


RN 211566-78-8 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)



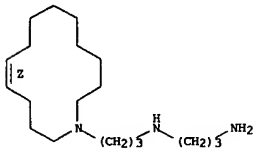
RN 211569-34-5 CAPLUS
CN 1,3-Propanediamine, N-[3-[(6Z)-azacyclopentadec-6-en-1-yl]propyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 398144-67-7 CAPLUS
CN 1,3-Propanediamine, N-[3-(5Z)-azacyclotetradec-5-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

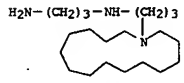
Double bond geometry as shown.



L5 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

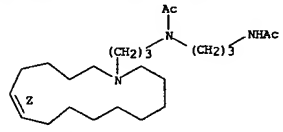
IT **211569-33-4**, Dihydromotuporamine C **251349-16-3**, Diacetyl motuporamine C **385437-34-3** **397262-93-0**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antiangiogenic macrocyclic amines and assays for inhibitors of cell invasion)

RN 211569-33-4 CAPLUS
CN 1,3-Propanediamine, N-[3-(azacyclopentadec-1-yl)propyl]- (9CI) (CA INDEX NAME)



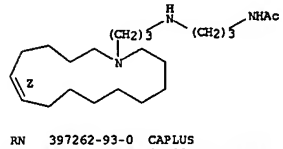
RN 251349-16-3 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 385437-34-3 CAPLUS
CN Acetamide, N-[3-[[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]amino]propyl]- (9CI) (CA INDEX NAME)

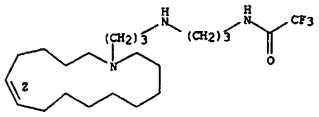
Double bond geometry as shown.



RN 397262-93-0 CAPLUS
CN Acetamide, N-[3-[[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]amino]propyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L5 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:893633 CAPLUS
DOCUMENT NUMBER: 136:164301
TITLE: Motuporamines, anti-invasion and anti-angiogenic alkaloids from the marine sponge Xestospongia exigua (Kirkpatrick): Isolation, structure elucidation, analogue synthesis, and conformational analysis
AUTHOR(5): Williams, David E.; Craig, Kyle S.; Patrick, Brian; McHardy, Lianne M.; van Soest, Rob; Roberge, Michel; Andersen, Raymond J.
CORPORATE SOURCE: Departments of Chemistry Oceanography (EOS) Biochemistry and Molecular Biology, University of British Columbia, Vancouver, BC, Can.
SOURCE: Journal of Organic Chemistry (2002), 67(1), 245-258 CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

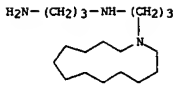
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Exts. of the sponge Xestospongia exigua collected in Papua New Guinea were pos. in a new assay for anti-invasion activity. Bioassay-guided fractionation led to the identification of the three known motuporamines A, B, and C along with the new motuporamines D (e.g. I), E, and F and a mixt. of G, H, and I. Motuporamines A, B, and C and the mixt. of G, H, and I were responsible for the anti-invasion activity of the crude ext. Motuporamine C has also been found to be anti-angiogenic. A series of analogs of the motuporamines have been synthesized and evaluated for anti-invasive activity. These SAR results revealed that a satd. 15-membered cyclic amine fused to the natural motuporamine diamine side chain (II) represented the optimal structure for anti-invasive activity in this family. Single-crystal X-ray diffraction anal. of one of the analogs (III) showed that in the solid state its 16-membered macrocyclic amine fragment adopted the [4444] quadrangular conformation predicted by calcns. to be the lowest energy conformation for the corresponding cycloalkane, cyclohexadecane. These data along with literature X-ray data and conformational anal. for derivs. of azacyclotridecane have been used as precedents for predicting the lowest energy ring conformations of other motuporamines. The SAR data from the natural and synthetic motuporamines have been combined with the conformational analyses to provide an outline of the functionality and shape required for activity in this family of alkaloids and to design a new analog (IV) that showed good anti-invasion activity.

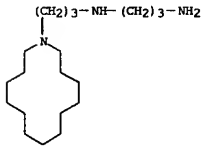
IT **211566-77-7**, Motuporamine A **211566-78-8**, Motuporamine B **211569-34-5**, Motuporamine C
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); BIOL (Biological study)
(anti-invasion and anti-angiogenic alkaloids from marine sponge Xestospongia exigua)

RN 211566-77-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX

L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
NAME)

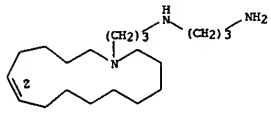


RN 211566-78-8 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)



RN 211569-34-5 CAPLUS
CN 1,3-Propanediamine, N-[3-[(6Z)-azacyclopentadec-6-en-1-yl]propyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

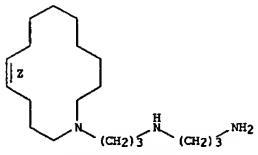


IT **398144-67-7P**, Motuporamine D **398144-69-9P**, Motuporamine F **398144-70-2P**, Motuporamine G **398144-76-8P**, Motuporamine H **398144-77-9P**, Motuporamine I
RL: NPO (Natural product occurrence); PAC (Pharmacological activity); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(anti-invasion and anti-angiogenic alkaloids from marine sponge Xestospongia exigua)

RN 398144-67-7 CAPLUS
CN 1,3-Propanediamine, N-[3-(5Z)-azacyclotetradec-5-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

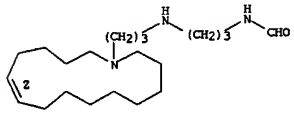
Double bond geometry as shown.

L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

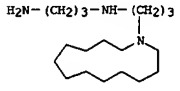


RN 398144-69-9 CAPLUS
CN Formamide, N-[3-[[3-(6Z)-azacyclotridec-6-en-1-ylpropyl]amino]propyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



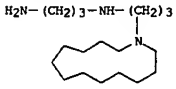
RN 398144-70-2 CAPLUS
CN 1,3-Propanediamine, N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



D1—Me

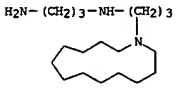
RN 398144-76-8 CAPLUS
CN 1,3-Propanediamine, N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



D1—Me

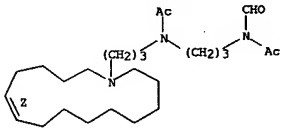
RN 398144-77-9 CAPLUS
CN 1,3-Propanediamine, N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



D1—Me

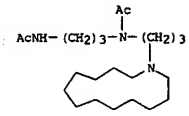
IT **397262-94-1P**, Diacetylmotuporamine F **398144-71-3P**, DiacetylMotuporamine G **398144-75-7P**, Diacetylmotuporamine H **398144-78-0P**, Diacetylmotuporamine I
RL: PRP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)
(anti-invasion and anti-angiogenic alkaloids from marine sponge Xestospongia exigua)
RN 397262-94-1 CAPLUS
CN Acetamide, N-[3-[acetyl[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]amino]propyl]-N-formyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



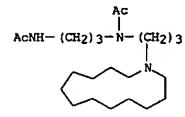
RN 398144-71-3 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



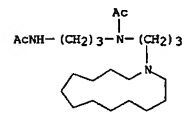
D1—Me

RN 398144-75-7 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



D1—Me

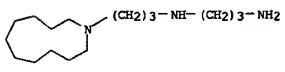
RN 398144-78-0 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



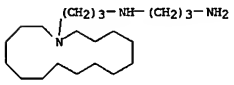
D1—Me

IT **397263-03-5P 397263-04-6P 397263-05-7P 397263-06-8P 397263-07-9P 397263-15-9P**, Azacyclotridecane-1-propanamine **397263-63-7P 397263-68-2P 397263-70-6P 397263-72-8P**

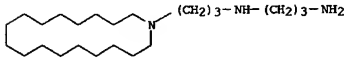
L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
397263-74-0P 397263-76-2P 397263-77-3P 397263-79-5P 397263-80-8P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(anti-invasive and antitumor activities of motuporamines and their analogs)
RN 397263-03-5 CAPLUS
CN 1,3-Propanediamine, N-(3-azacycloundec-1-ylpropyl)- (9CI) (CA INDEX NAME)



RN 397263-04-6 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclohexadec-1-ylpropyl)- (9CI) (CA INDEX NAME)

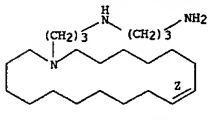


RN 397263-05-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclooctadec-1-ylpropyl)- (9CI) (CA INDEX NAME)



RN 397263-06-8 CAPLUS
CN 1,3-Propanediamine, N-[3-(8Z)-azacyclooctadec-8-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

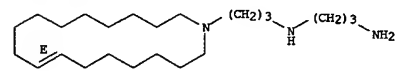
Double bond geometry as shown.



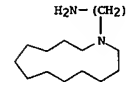
RN 397263-07-9 CAPLUS
CN 1,3-Propanediamine, N-[3-(8E)-azacyclooctadec-8-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

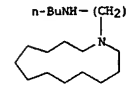
L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



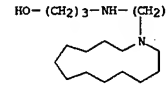
RN 397263-15-9 CAPLUS
CN Azacyclotridecane-1-propanamine (9CI) (CA INDEX NAME)



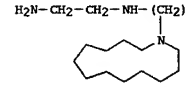
RN 397263-63-7 CAPLUS
CN Azacyclotridecane-1-propanamine, N-butyl- (9CI) (CA INDEX NAME)



RN 397263-68-2 CAPLUS
CN 1-Propanol, 3-[(3-azacyclotridec-1-ylpropyl)amino]- (9CI) (CA INDEX NAME)

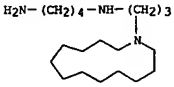


RN 397263-70-6 CAPLUS
CN 1,2-Ethanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)

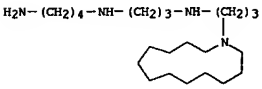


RN 397263-72-8 CAPLUS
CN 1,4-Butanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)

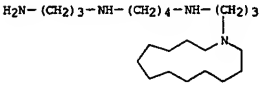
L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



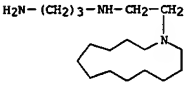
RN 397263-74-0 CAPLUS
CN 1,4-Butanediamine, N-[3-[(3-azacyclotridec-1-ylpropyl)amino]propyl]- (9CI) (CA INDEX NAME)



RN 397263-76-2 CAPLUS
CN 1,4-Butanediamine, N-(3-aminopropyl)-N'-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)



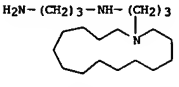
RN 397263-77-3 CAPLUS
CN 1,3-Propanediamine, N-(2-azacyclotridec-1-ylethyl)- (9CI) (CA INDEX NAME)



RN 397263-79-5 CAPLUS
CN 1,3-Propanediamine, N-(4-azacyclotridec-1-ylbutyl)- (9CI) (CA INDEX NAME)

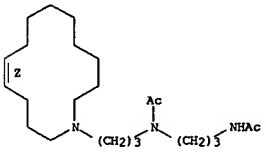
L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

IT 211569-33-4P, Dihydromotuporamine C
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and anti-invasive activity of)
RN 211569-33-4 CAPLUS
CN 1,3-Propanediamine, N-[3-(azacyclopentadec-1-yl)propyl]- (9CI) (CA INDEX NAME)

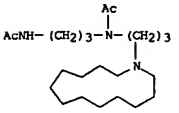


IT 397263-01-3P, Diacetylmotuporamine D
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and properties of)
RN 397263-01-3 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(5Z)-azacyclotetradec-5-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

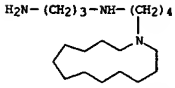


IT 211388-13-5P, Diacetylmotuporamine A 211388-14-6P, Diacetylmotuporamine B 251349-16-3P, Diacetylmotuporamine C
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 211388-13-5 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)

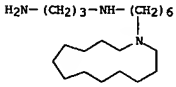


RN 211388-14-6 CAPLUS

L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

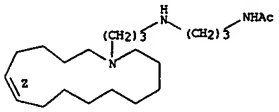


RN 397263-80-8 CAPLUS
CN 1,3-Propanediamine, N-(6-azacyclotridec-1-ylhexyl)- (9CI) (CA INDEX NAME)



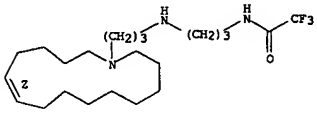
IT 385437-34-3 397262-93-0
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(artifact from marine sponge Xestospongia exigua)
RN 385437-34-3 CAPLUS
CN Acetamide, N-[3-[[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]amino]propyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

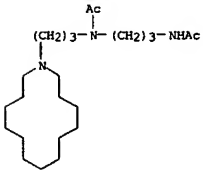


RN 397262-93-0 CAPLUS
CN Acetamide, N-[3-[[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]amino]propyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

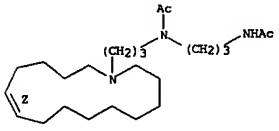


L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
CN Acetamide, N-[3-(acetylamino)propyl]-N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)



RN 251349-16-3 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



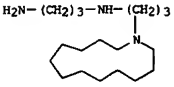
REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:712129 CAPLUS
DOCUMENT NUMBER: 136:63714
TITLE: Inhibition of tumor cell invasion and **angiogenesis** by motuporamines
AUTHOR(S): Roskelley, Calvin D.; Williams, David E.; McHardy, Lianne M.; Leong, Kevin G.; Troussard, Armelle; Karsan, Aly; Andersen, Raymond J.; Dedhar, Shoukat; Roberge, Michel
CORPORATE SOURCE: Departments of Anotomy, University of British Columbia, Vancouver, BC, V6T 1Z3, Can.
SOURCE: Cancer Research (2001), 61(18), 6788-6794
CODEN: CNREA8; ISSN: 0008-5472
PUBLISHER: American Association for Cancer Research
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Tissue invasion is an important determinant of **angiogenesis** and metastasis and constitutes an attractive target for cancer therapy. We have developed an assay to identify agents that inhibit invasion by mechanisms other than inhibition of cell attachment or cytotoxicity. A screen of marine sponge exts. identified motuporamines as micromolar inhibitors of invasion of basement membrane gels by MDA-231 breast carcinoma, PC-3 prostate carcinoma, and U-87 and U-251 glioma cells. Motuporamine C inhibits cell migration in monolayer cultures and impairs actin-mediated membrane ruffling at the leading edge of lamellae. Motuporamine C also reduces .beta.1-integrin activation, raising the possibility that it interferes with "inside-out" signaling to integrins. In addn., motuporamine C inhibits **angiogenesis** in an in vitro sprouting assay with human endothelial cells and an in vivo chick chorioallantoic membrane assay. The motuporamines show little or no toxicity or inhibition of cell proliferation, and they are structurally simple and easy to synthesize, making them attractive drug candidates.

IT **211566-77-7**, Motuporamine A **211569-34-5**, Motuporamine C **251349-16-3 385437-34-3**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(inhibition of tumor cell invasion and **angiogenesis** by motuporamines)

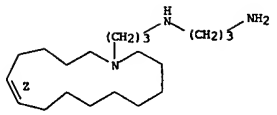
RN 211566-77-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)



RN 211569-34-5 CAPLUS
CN 1,3-Propanediamine, N-[3-[(6Z)-azacyclopentadec-6-en-1-yl]propyl]- (9CI) (CA INDEX NAME)

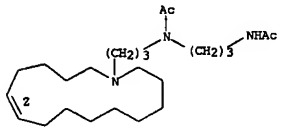
Double bond geometry as shown.

L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



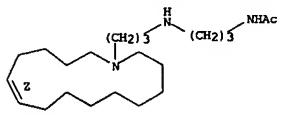
RN 251349-16-3 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 385437-34-3 CAPLUS
CN Acetamide, N-[3-[[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]amino]propyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d l4 ibib abs hitstr tot

L4 ANSWER 1 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:574910 CAPLUS
DOCUMENT NUMBER: 137:119652
TITLE: Antiangiogenic compounds and an assay for inhibitors of cell invasion
INVENTOR(S): Roskelley, Calvin; Andersen, Raymond; Williams, David; Roberge, Michel; Dedhar, Shoukat; Karsan, Aly; Minchinton, Andrew
PATENT ASSIGNEE(S): The University of British Columbia, Can.
SOURCE: PCT Int. Appl., 56 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002058679	A2	20020801	WO 2002-CA97	20020125
WO 2002058679	A3	20030515		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003004149	A1	20030102	US 2002-57846	20020125
PRIORITY APPLN. INFO.:			CA 2001-2332138 A	20010125
			US 2001-330670P P	20011026

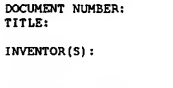
OTHER SOURCE(S): MARPAT 137:119652

AB This invention provides the use of macrocyclic amines for inhibition of cellular invasion or angiogenesis. Compds. and pharmaceutical compns. of this invention are useful in the treatment of conditions characterized by cellular invasion or angiogenesis, including cancer. Compds. that may be used in this invention include the motuporamines, which are isolated from methanol exts. of Xestospongia exigua.

IT **398144-70-2**, Motuporamine G **398144-76-8**, Motuporamine H
398144-77-9, Motuporamine I
RL: NPO (Natural product occurrence); BIOL (Biological study); OCCU (Occurrence)
(antiangiogenic macrocyclic amines and assays for inhibitors of cell invasion)

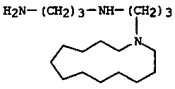
RN 398144-70-2 CAPLUS
CN 1,3-Propanediamine, N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



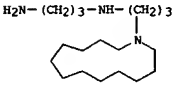
D1-Me

RN 398144-76-8 CAPLUS
CN 1,3-Propanediamine, N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



D1-Me

RN 398144-77-9 CAPLUS
CN 1,3-Propanediamine, N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

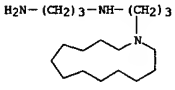


D1-Me

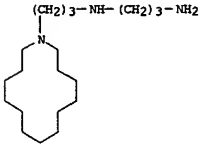
IT **211566-77-7**, Motuporamine A **211566-78-8**, Motuporamine B
211569-34-5, Motuporamine C **398144-67-7**, Motuporamine D
RL: NPO (Natural product occurrence); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES (Uses)
(antiangiogenic macrocyclic amines and assays for inhibitors of cell invasion)

RN 211566-77-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

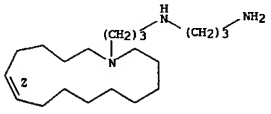


RN 211566-78-8 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)



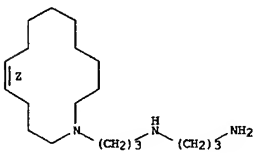
RN 211569-34-5 CAPLUS
CN 1,3-Propanediamine, N-[3-[(6Z)-azacyclopentadec-6-en-1-yl]propyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 398144-67-7 CAPLUS
CN 1,3-Propanediamine, N-[3-(5Z)-azacyclotetradec-5-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

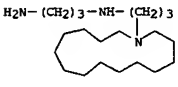
Double bond geometry as shown.



L4 ANSWER 1 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

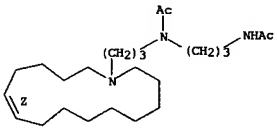
IT **211569-33-4**, Dihydromotuporamine C **251349-16-3**, Diacetyl motuporamine C **385437-34-3** **397262-93-0**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antiangiogenic macrocyclic amines and assays for inhibitors of cell invasion)

RN 211569-33-4 CAPLUS
CN 1,3-Propanediamine, N-[3-(azacyclopentadec-1-yl)propyl]- (9CI) (CA INDEX NAME)



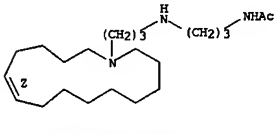
RN 251349-16-3 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 385437-34-3 CAPLUS
CN Acetamide, N-[3-[[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]amino]propyl]- (9CI) (CA INDEX NAME)

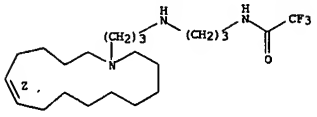
Double bond geometry as shown.



RN 397262-93-0 CAPLUS
CN Acetamide, N-[3-[[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]amino]propyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 1 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



L4 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:893633 CAPLUS
DOCUMENT NUMBER: 136:164301
TITLE: Motuporamines, anti-invasion and anti-angiogenic alkaloids from the marine sponge Xestospongia exigua (Kirkpatrick): Isolation, structure elucidation, analogue synthesis, and conformational analysis
AUTHOR(S): Williams, David E.; Craig, Kyle S.; Patrick, Brian; McHardy, Lianne M.; van Soest, Rob; Roberge, Michel; Andersen, Raymond J.
CORPORATE SOURCE: Departments of Chemistry Oceanography (EOS) Biochemistry and Molecular Biology, University of British Columbia, Vancouver, BC, Can.
SOURCE: Journal of Organic Chemistry (2002), 67(1), 245-258 CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

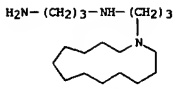
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Exts. of the sponge Xestospongia exigua collected in Papua New Guinea were pos. in a new assay for anti-invasion activity. Bioassay-guided fractionation led to the identification of the three known motuporamines A , B, and C along with the new motuporamines D (e.g. I), E, and F and a mixt. of G, H, and I. Motuporamines A, B, and C and the mixt. of G, H, and I were responsible for the anti-invasion activity of the crude ext. Motuporamine C has also been found to be anti-angiogenic. A series of analogs of the motuporamines have been synthesized and evaluated for anti-invasive activity. These SAR results revealed that a satd. 15-membered cyclic amine fused to the natural motuporamine diamine side chain (II) represented the optimal structure for anti-invasive activity in this family. Single-crystal X-ray diffraction anal. of one of the analogs (III) showed that in the solid state its 16-membered macrocyclic amine fragment adopted the [4444] quadrangular conformation predicted by calcns. to be the lowest energy conformation for the corresponding cycloalkane, cyclohexadecane. These data along with literature X-ray data and conformational anal. for derivs. of azacyclotridecane have been used as precedents for predicting the lowest energy ring conformations of other motuporamines. The SAR data from the natural and synthetic motuporamines have been combined with the conformational analyses to provide an outline of the functionality and shape required for activity in this family of alkaloids and to design a new analog (IV) that showed good anti-invasion activity.

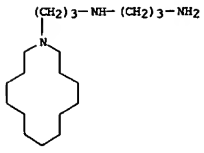
IT **211566-77-7**, Motuporamine A **211566-78-8**, Motuporamine B **211569-34-5**, Motuporamine C
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); BIOL (Biological study)
(anti-invasion and anti-angiogenic alkaloids from marine sponge Xestospongia exigua)

RN 211566-77-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX

L4 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
NAME)

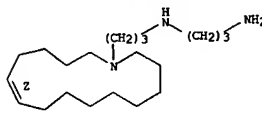


RN 211566-78-8 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)



RN 211569-34-5 CAPLUS
CN 1,3-Propanediamine, N-[3-[(6Z)-azacyclopentadec-6-en-1-yl]propyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

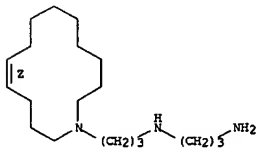


IT **398144-67-7P**, Motuporamine D **398144-69-9P**, Motuporamine F **398144-70-2P**, Motuporamine G **398144-76-8P**, Motuporamine H **398144-77-9P**, Motuporamine I
RL: NPO (Natural product occurrence); PAC (Pharmacological activity); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(anti-invasion and anti-angiogenic alkaloids from marine sponge Xestospongia exigua)

RN 398144-67-7 CAPLUS
CN 1,3-Propanediamine, N-[3-(5Z)-azacyclotetradec-5-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

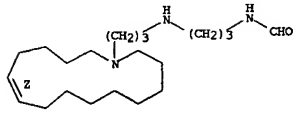
Double bond geometry as shown.

L4 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

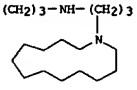


RN 398144-69-9 CAPLUS
CN Formamide, N-[3-[[3-(6Z)-azacyclotridec-6-en-1-ylpropyl]amino]propyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



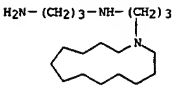
RN 398144-70-2 CAPLUS
CN 1,3-Propanediamine, N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



D1—Me

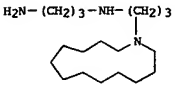
RN 398144-76-8 CAPLUS
CN 1,3-Propanediamine, N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



D1—Me

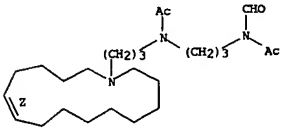
RN 398144-77-9 CAPLUS
CN 1,3-Propanediamine, N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



D1—Me

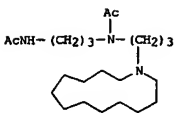
IT **397262-94-1P**, Diacetylmotuporamine F **398144-71-3P**, DiacetylMotuporamine G **398144-75-7P**, Diacetylmotuporamine H **398144-78-0P**, Diacetylmotuporamine I
RL: PRP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)
(anti-invasion and anti-angiogenic alkaloids from marine sponge Xestospongia exigua)
RN 397262-94-1 CAPLUS
CN Acetamide, N-[3-[acetyl[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]amino]propyl]-N-formyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



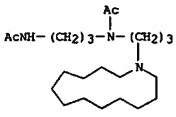
RN 398144-71-3 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



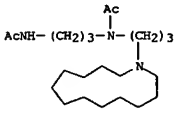
D1—Me

RN 398144-75-7 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



D1—Me

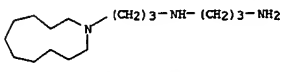
RN 398144-78-0 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



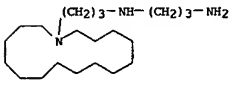
D1—Me

IT **397263-03-5P 397263-04-6P 397263-05-7P 397263-06-8P 397263-07-9P 397263-15-9P**, Azacyclotridecane-1-propanamine **397263-63-7P 397263-68-2P 397263-70-6P 397263-72-8P**

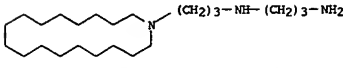
L4 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
397263-74-0P 397263-76-2P 397263-77-3P 397263-79-5P 397263-80-8P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(anti-invasive and antitumor activities of motuporamines and their analogs)
RN 397263-03-5 CAPLUS
CN 1,3-Propanediamine, N-(3-azacycloundec-1-ylpropyl)- (9CI) (CA INDEX NAME)



RN 397263-04-6 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclohexadec-1-ylpropyl)- (9CI) (CA INDEX NAME)

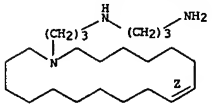


RN 397263-05-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclooctadec-1-ylpropyl)- (9CI) (CA INDEX NAME)



RN 397263-06-8 CAPLUS
CN 1,3-Propanediamine, N-[3-(8Z)-azacyclooctadec-8-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

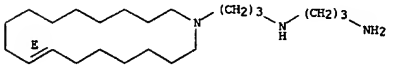
Double bond geometry as shown.



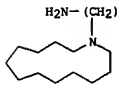
RN 397263-07-9 CAPLUS
CN 1,3-Propanediamine, N-[3-(8E)-azacyclooctadec-8-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

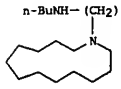
L4 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



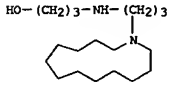
RN 397263-15-9 CAPLUS
CN Azacyclotridecane-1-propanamine (9CI) (CA INDEX NAME)



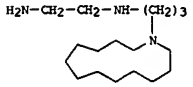
RN 397263-63-7 CAPLUS
CN Azacyclotridecane-1-propanamine, N-butyl- (9CI) (CA INDEX NAME)



RN 397263-68-2 CAPLUS
CN 1-Propanol, 3-[(3-azacyclotridec-1-ylpropyl)amino]- (9CI) (CA INDEX NAME)

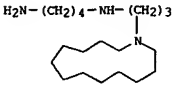


RN 397263-70-6 CAPLUS
CN 1,2-Ethanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)

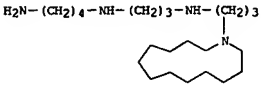


RN 397263-72-8 CAPLUS
CN 1,4-Butanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)

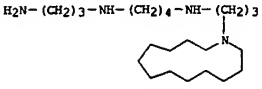
L4 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



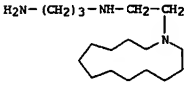
RN 397263-74-0 CAPLUS
CN 1,4-Butanediamine, N-[3-[(3-azacyclotridec-1-ylpropyl)amino]propyl]- (9CI) (CA INDEX NAME)



RN 397263-76-2 CAPLUS
CN 1,4-Butanediamine, N-(3-aminopropyl)-N'-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)

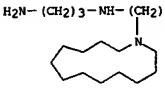


RN 397263-77-3 CAPLUS
CN 1,3-Propanediamine, N-(2-azacyclotridec-1-ylethyl)- (9CI) (CA INDEX NAME)

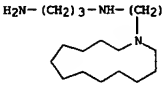


RN 397263-79-5 CAPLUS
CN 1,3-Propanediamine, N-(4-azacyclotridec-1-ylbutyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

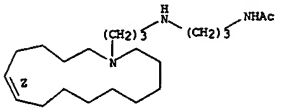


RN 397263-80-8 CAPLUS
CN 1,3-Propanediamine, N-(6-azacyclotridec-1-ylhexyl)- (9CI) (CA INDEX NAME)



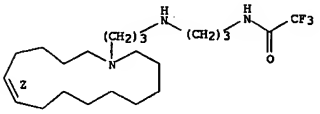
IT 385437-34-3 397262-93-0
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(artifact from marine sponge Xestospongia exigua)
RN 385437-34-3 CAPLUS
CN Acetamide, N-[3-[[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]amino]propyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



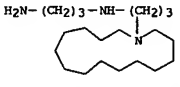
RN 397262-93-0 CAPLUS
CN Acetamide, N-[3-[[3-(62)-azacyclopentadec-6-en-1-ylpropyl]amino]propyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



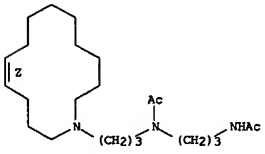
L4 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

IT 211569-33-4P, Dihydromotuporamine C
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and anti-invasive activity of)
RN 211569-33-4 CAPLUS
CN 1,3-Propanediamine, N-[3-(azacyclopentadec-1-yl)propyl]- (9CI) (CA INDEX NAME)

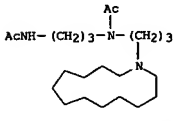


IT 397263-01-3P, Diacetylmotuporamine D
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and properties of)
RN 397263-01-3 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(5Z)-azacyclotetradec-5-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

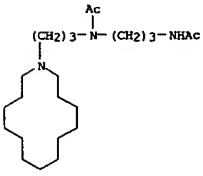


IT 211388-13-5P, Diacetylmotuporamine A 211388-14-6P, Diacetylmotuporamine B 251349-16-3P, Diacetylmotuporamine C
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 211388-13-5 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)



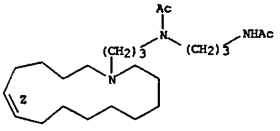
RN 211388-14-6 CAPLUS

L4 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
CN Acetamide, N-[3-(acetylamino)propyl]-N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)



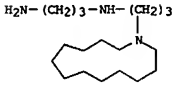
RN 251349-16-3 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

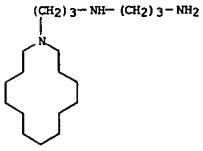


REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:883060 CAPLUS
DOCUMENT NUMBER: 137:185705
TITLE: Application of ring-closing metathesis to the synthesis of unsaturated 14-membered lactams and the marine alkaloids motuporamines A-C
AUTHOR(S): Goldring, William Peter Donald
CORPORATE SOURCE: Univ. of British Columbia, Vancouver, BC, Can.
SOURCE: (2000) 370 pp. Avail.: UMI, Order No. DANQ56551
From: Diss. Abstr. Int., B 2001, 61(12), 6477
DOCUMENT TYPE: Dissertation
LANGUAGE: English
AB Unavailable
IT 211566-77-7P, Motuporamine A 211566-78-8P, Motuporamine B 211569-34-5P, Motuporamine C
RL: PNU (Preparation, unclassified); PREP (Preparation)
(application of ring-closing metathesis to synthesis of unsatd. 14-membered lactams and marine alkaloids motuporamines A-C)
RN 211566-77-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)



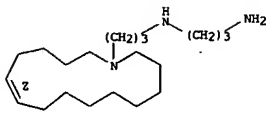
RN 211566-78-8 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)



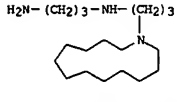
RN 211569-34-5 CAPLUS
CN 1,3-Propanediamine, N-[3-[(6Z)-azacyclopentadec-6-en-1-yl]propyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 3 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



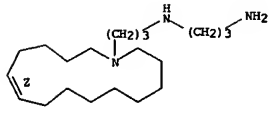
L4 ANSWER 4 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:712129 CAPLUS
DOCUMENT NUMBER: 136:63714
TITLE: Inhibition of tumor cell invasion and angiogenesis by motuporamines
AUTHOR(S): Roskelley, Calvin D.; Williams, David E.; McHardy, Lianne M.; Leong, Kevin G.; Troussard, Armelle; Karsan, Aly; Andersen, Raymond J.; Dedhar, Shoukat; Roberge, Michel
CORPORATE SOURCE: Departments of Anotomy, University of British Columbia, Vancouver, BC, V6T 1Z3, Can.
SOURCE: Cancer Research (2001), 61(18), 6788-6794
CODEN: CNREA8; ISSN: 0008-5472
PUBLISHER: American Association for Cancer Research
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Tissue invasion is an important determinant of angiogenesis and metastasis and constitutes an attractive target for cancer therapy. We have developed an assay to identify agents that inhibit invasion by mechanisms other than inhibition of cell attachment or cytotoxicity. A screen of marine sponge exts. identified motuporamines as micromolar inhibitors of invasion of basement membrane gels by MDA-231 breast carcinoma, PC-3 prostate carcinoma, and U-87 and U-251 glioma cells. Motuporamine C inhibits cell migration in monolayer cultures and impairs actin-mediated membrane ruffling at the leading edge of lamellae. Motuporamine C also reduces .beta.1-integrin activation, raising the possibility that it interferes with "inside-out" signaling to integrins. In addn., motuporamine C inhibits angiogenesis in an in vitro sprouting assay with human endothelial cells and an in vivo chick chorioallantoic membrane assay. The motuporamines show little or no toxicity or inhibition of cell proliferation, and they are structurally simple and easy to synthesize, making them attractive drug candidates.
IT 211566-77-7, Motuporamine A 211569-34-5, Motuporamine C 251349-16-3 385437-34-3
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(inhibition of tumor cell invasion and angiogenesis by motuporamines)
RN 211566-77-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)



RN 211569-34-5 CAPLUS
CN 1,3-Propanediamine, N-[3-[(6Z)-azacyclopentadec-6-en-1-yl]propyl]- (9CI) (CA INDEX NAME)

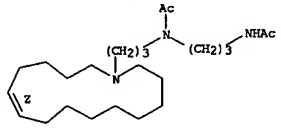
Double bond geometry as shown.

L4 ANSWER 4 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



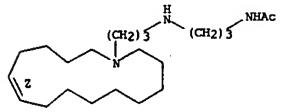
RN 251349-16-3 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



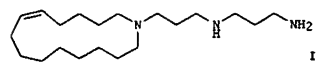
RN 385437-34-3 CAPLUS
CN Acetamide, N-[3-[[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]amino]propyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

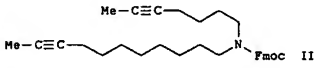


REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:191704 CAPLUS
DOCUMENT NUMBER: 133:43691
TITLE: Ring-Closing Alkyne Metathesis. Stereoselective Synthesis of the Cytotoxic Marine Alkaloid Motuporamine C
AUTHOR(S): Fuerstner, Alois; Rumbo, Antonio
CORPORATE SOURCE: Max-Planck-Institut fuer Kohlenforschung, Muelheim/Ruhr, D-45470, Germany
SOURCE: Journal of Organic Chemistry (2000), 65(8), 2608-2611 CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:43691
GI



I



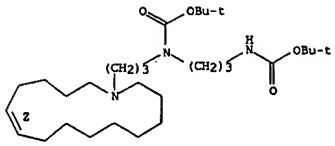
II

AB Motuporamine C (I) was synthesized from MeC.tplbond.C(CH2)8OH in 8 steps via ring-closing alkyne metathesis of the undecynylheptynylamine II followed by alkylation.
IT **274675-60-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective synthesis of the cytotoxic marine alkaloid motuporamine C)
RN 274675-60-4 CAPLUS
CN Carbamic acid, [3-(6Z)-azacyclopentadec-6-en-1-ylpropyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

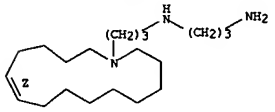
L4 ANSWER 5 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

L4 ANSWER 5 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



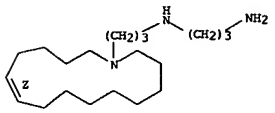
IT **211569-34-5P 274675-69-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective synthesis of the cytotoxic marine alkaloid motuporamine C)
RN 211569-34-5 CAPLUS
CN 1,3-Propanediamine, N-[3-[(6Z)-azacyclopentadec-6-en-1-yl]propyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 274675-69-3 CAPLUS
CN 1,3-Propanediamine, N-[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]-, dihydrochloride (9CI) (CA INDEX NAME)

Double bond geometry as shown.

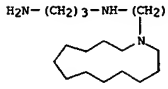


●2 HCl

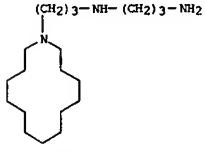
REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

L4 ANSWER 6 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:715619 CAPLUS
DOCUMENT NUMBER: 132:122787
TITLE: Cytotoxic alkaloids motuporamines A-C, synthesis and structural verification. [Erratum to document cited in CA132:12426]
AUTHOR(S): Goldring, William P. D.; Weiler, Larry
CORPORATE SOURCE: Dep. Chemistry, Univ. British Columbia, Vancouver, BC, V6T 1Z1, Can.
SOURCE: Organic Letters (1999), 1(11), 1874 CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The cor. ref. 2 should read as follows: "(2) Baldwin, J. E.; Vollmer, H. R.; Lee, V. Tetrahedron Lett. 1999, 40, 5401.".
IT **211566-77-7P**, Motuporamine A **211566-78-8P**, Motuporamine B
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(cytotoxic alkaloids motuporamines A-C, synthesis and structural verification (Erratum))
RN 211566-77-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)

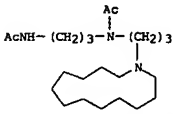


RN 211566-78-8 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)

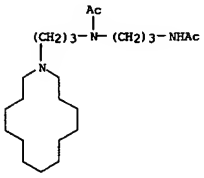


IT **211388-13-5P 211388-14-6P 211569-34-5P**, Motuporamine C **251349-16-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(cytotoxic alkaloids motuporamines A-C, synthesis and structural verification (Erratum))
RN 211388-13-5 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 6 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

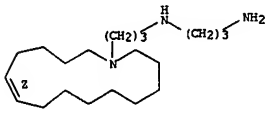


RN 211388-14-6 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)



RN 211569-34-5 CAPLUS
CN 1,3-Propanediamine, N-[3-[(6Z)-azacyclopentadec-6-en-1-yl]propyl]- (9CI) (CA INDEX NAME)

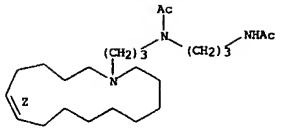
Double bond geometry as shown.



RN 251349-16-3 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

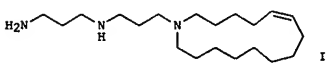
Double bond geometry as shown.

L4 ANSWER 6 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



L4 ANSWER 7 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN

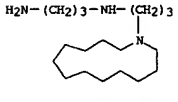
ACCESSION NUMBER: 1999:629478 CAPLUS
DOCUMENT NUMBER: 132:12426
TITLE: Cytotoxic Alkaloids Motuporamines A-C: Synthesis and Structural Verification
AUTHOR(S): Goldring, William P. D.; Weiler, Larry
CORPORATE SOURCE: Department of Chemistry, University of British Columbia, Vancouver, BC, V6T 1Z1, Can.
SOURCE: Organic Letters (1999), 1(9), 1471-1473
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:12426
GI



AB The unusual structure and biol. properties of the marine alkaloids motuporamines A-C, as well as the uncertainty as to the position of the olefin within the ring of motuporamine C, led to the synthesis of these compds. The strategy utilized the ring-closing metathesis reaction to form the 14- and 15-membered rings and Michael addn. and amidation chem. to introduce the spermine-like unit. The syntheses, structure assignment verifications, and also the detn. of the position of the olefin in motuporamine C (I) are described.

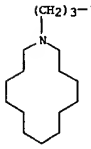
IT **211566-77-7P**, Motuporamine A **211566-78-8P**, Motuporamine B
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(cytotoxic alkaloids motuporamines A-C, synthesis and structural verification)

RN 211566-77-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)



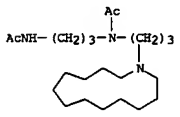
RN 211566-78-8 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 7 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

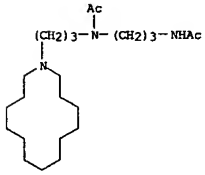


IT **211388-13-5P 211388-14-6P 211569-34-5P**, Motuporamine C **251349-16-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(cytotoxic alkaloids motuporamines A-C, synthesis and structural verification)

RN 211388-13-5 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)



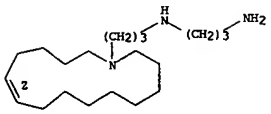
RN 211388-14-6 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)



RN 211569-34-5 CAPLUS
CN 1,3-Propanediamine, N-[3-[(6Z)-azacyclopentadec-6-en-1-yl]propyl]- (9CI) (CA INDEX NAME)

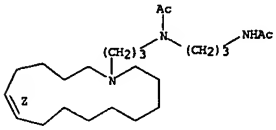
Double bond geometry as shown.

L4 ANSWER 7 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



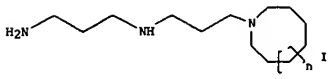
RN 251349-16-3 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

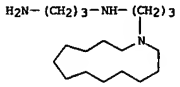


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:448471 CAPLUS
DOCUMENT NUMBER: 131:257741
TITLE: Total synthesis of cytotoxic sponge alkaloids motuporamines A and B
AUTHOR(S): Baldwin, Jack E.; Vollmer, Heidi R.; Lee, Victor
CORPORATE SOURCE: The Dyson Perrins Laboratory, University of Oxford, Oxford, OX1 3QY, UK
SOURCE: Tetrahedron Letters (1999), 40(29), 5401-5404
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:257741
GI

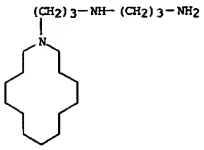


AB The synthesis of two sponge alkaloids, motuporamines A and B (I) (n = 6, 7) is reported. The key step involved a reductive amination using sodium triacetoxyborohydride.
IT **211566-77-7P 211566-78-8P 245119-67-9P**
245119-68-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(total synthesis of cytotoxic sponge alkaloids motuporamines A and B)
RN 211566-77-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)

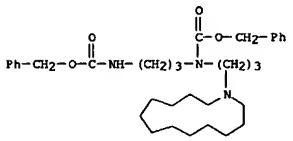


RN 211566-78-8 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)

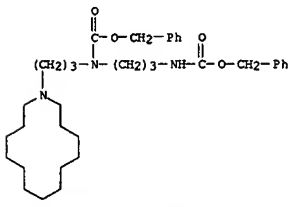
L4 ANSWER 8 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



RN 245119-67-9 CAPLUS
CN Carbamic acid, (3-azacyclotridec-1-ylpropyl)[3-[[(phenylmethoxy)carbonyl]amino]propyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

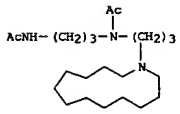


RN 245119-68-0 CAPLUS
CN Carbamic acid, (3-azacyclotetradec-1-ylpropyl)[3-[[(phenylmethoxy)carbonyl]amino]propyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

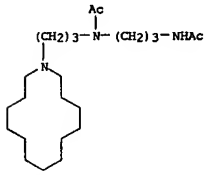


IT **211388-13-5P 211388-14-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of cytotoxic sponge alkaloids motuporamines A and B)
RN 211388-13-5 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 8 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

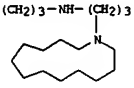


RN 211388-14-6 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)



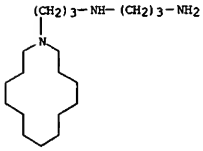
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1998:446771 CAPLUS
DOCUMENT NUMBER: 129:173061
TITLE: Motuporamines A-C, Cytotoxic Alkaloids Isolated from the Marine Sponge Xestospongia exigua (Kirkpatrick)
AUTHOR(S): Williams, David E.; Lassota, Peter; Andersen, Raymond J.
CORPORATE SOURCE: Departments of Chemistry and Oceanography Earth Ocean Sciences, University of British Columbia, Vancouver, BC, V6T 1Z1, Can.
SOURCE: Journal of Organic Chemistry (1998), 63(14), 4838-4841 CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Bioassay guided fractionation of the Xestospongia exigua exts. yielded a mixt. of motuporamines A-C, which contain a spermidine-like substructure and represent a new family of cytotoxic sponge alkaloids. The motuporamines A-C were diacetylated and sepd. via reversed phase HPLC. NMR data for the motuporamines and their diacetates was detailed.
IT **211566-77-7P**, Motuporamine A **211566-78-8P**, Motuporamine B **211569-34-5P**, Motuporamine C
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(isolation of motuporamines A-C, cytotoxic alkaloids, from the marine sponge Xestospongia exigua)
RN 211566-77-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)



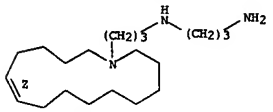
RN 211566-78-8 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 9 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

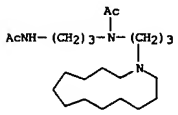


RN 211569-34-5 CAPLUS
CN 1,3-Propanediamine, N-[3-[(6Z)-azacyclopentadec-6-en-1-yl]propyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

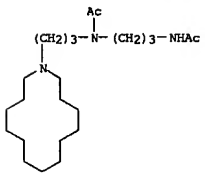


IT **211388-13-5P**, Diacetylmotuporamine A **211388-14-6P**, Diacetylmotuporamine B **251349-16-3P**, Diacetylmotuporamine C
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(isolation of motuporamines A-C, cytotoxic alkaloids, from the marine sponge Xestospongia exigua)
RN 211388-13-5 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)



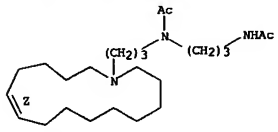
RN 211388-14-6 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 9 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



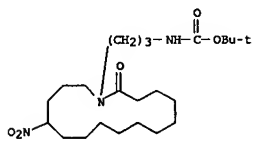
RN 251349-16-3 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

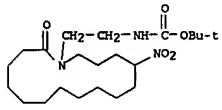


REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1994:77488 CAPLUS
DOCUMENT NUMBER: 120:77488
TITLE: The mass spectral loss of water from macrocyclic amino ketones
AUTHOR(S): Benz, Herbert; Hesse, Manfred
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, CH-8057, Switz.
SOURCE: Helvetica Chimica Acta (1993), 76(4), 1636-48 CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
AB Macrocyclic oxo-lactams contg. an aminoalkyl side chain are stable natural products. Their electron-impact mass spectra are characterized by intense [M - H2O]+ signals, the mol. ion signal itself is missing. Under electrospray ionization conditions, on the other hand, the [M + 1]+ ion is the only detected signal. The loss of water is explained in terms of an internal (thermal) Schiff-base formation, leading to, e.g., a bicyclo[11.9.4]-system. The alcs. corresponding to the macrocyclic ketones and/or lactams show expected mass-spectral behavior following well-known rules.
IT **99379-76-7P** **152450-40-3P** **152450-42-5P** **152450-43-6P** **152450-44-7P** **152450-45-8P** **152450-46-9P** **152450-47-0P** **152450-48-1P** **152450-49-2P** **152450-50-5P** **152450-51-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(intermediate in prepn. of aminoalkyl macrocyclic lactams)
RN 99379-76-7 CAPLUS
CN Carbamic acid, [3-(13-nitro-2-oxoazacyclohexadec-1-yl)propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

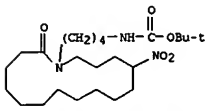


RN 152450-40-3 CAPLUS
CN Carbamic acid, [2-(13-nitro-2-oxoazacyclohexadec-1-yl)ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

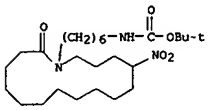


RN 152450-42-5 CAPLUS
CN Carbamic acid, [4-(13-nitro-2-oxoazacyclohexadec-1-yl)butyl]-,

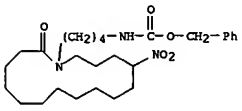
L4 ANSWER 10 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



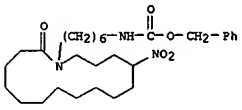
RN 152450-43-6 CAPLUS
CN Carbamic acid, [6-(13-nitro-2-oxoazacyclohexadec-1-yl)hexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 152450-44-7 CAPLUS
CN Carbamic acid, [4-(13-nitro-2-oxoazacyclohexadec-1-yl)butyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

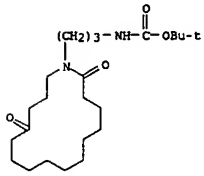


RN 152450-45-8 CAPLUS
CN Carbamic acid, [6-(13-nitro-2-oxoazacyclohexadec-1-yl)hexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

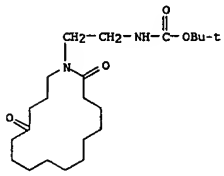


RN 152450-46-9 CAPLUS

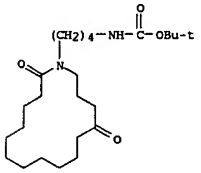
L4 ANSWER 10 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
CN Carbamic acid, [3-(2,13-dioxoazacyclohexadec-1-yl)propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 152450-47-0 CAPLUS
CN Carbamic acid, [2-(2,13-dioxoazacyclohexadec-1-yl)ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

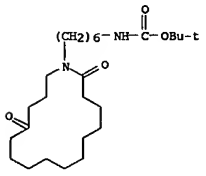


RN 152450-48-1 CAPLUS
CN Carbamic acid, [4-(2,13-dioxoazacyclohexadec-1-yl)butyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

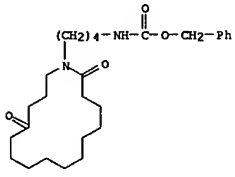


L4 ANSWER 10 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

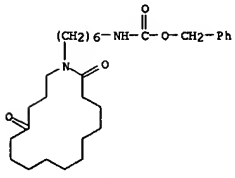
RN 152450-49-2 CAPLUS
CN Carbamic acid, [6-(2,13-dioxoazacyclohexadec-1-yl)hexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 152450-50-5 CAPLUS
CN Carbamic acid, [4-(2,13-dioxoazacyclohexadec-1-yl)butyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

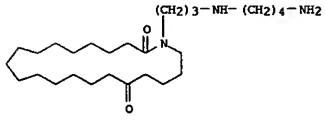


RN 152450-51-6 CAPLUS
CN Carbamic acid, [6-(2,13-dioxoazacyclohexadec-1-yl)hexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

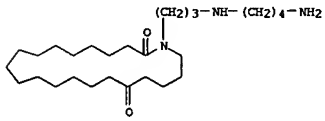


IT 152450-26-5

L4 ANSWER 10 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
RL: PRP (Properties)
(mass spectrum of)
RN 152450-26-5 CAPLUS
CN Azacycloheneicosane-2,17-dione, 1-[3-[(4-aminobutyl)amino]propyl]- (9CI) (CA INDEX NAME)

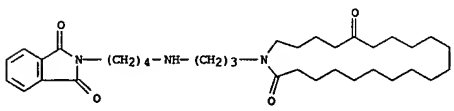


IT 152450-23-2 152450-24-3 152450-25-4
152450-29-8 152450-32-3 152450-34-5
152450-35-6
RL: PRP (Properties)
(mass spectrum of, water loss in)
RN 152450-23-2 CAPLUS
CN Azacycloheneicosane-2,17-dione, 1-[3-[(4-aminobutyl)amino]propyl]-, dihydrochloride (9CI) (CA INDEX NAME)



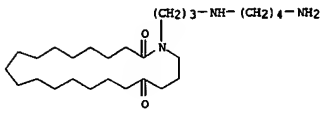
●2 HCl

RN 152450-24-3 CAPLUS
CN 1H-Isoindole-1,3(2H)-dione, 2-[4-[[3-(2,17-dioxoazacycloheneicos-1-yl)propyl]amino]butyl]-, monohydrochloride (9CI) (CA INDEX NAME)



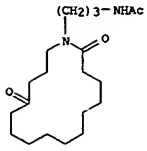
● HCl

L4 ANSWER 10 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
RN 152450-25-4 CAPLUS
CN Azacycloheneicosane-2,18-dione, 1-[3-[(4-aminobutyl)amino]propyl]-, dihydrochloride (9CI) (CA INDEX NAME)

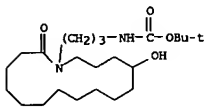


●2 HCl

RN 152450-29-8 CAPLUS
CN Acetamide, N-[3-(2,13-dioxoazacyclohexadec-1-yl)propyl]- (9CI) (CA INDEX NAME)

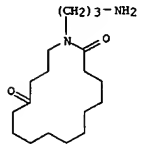


RN 152450-32-3 CAPLUS
CN Carbamic acid, [3-(13-hydroxy-2-oxoazacyclohexadec-1-yl)propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

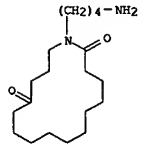


RN 152450-34-5 CAPLUS
CN Acetamide, N-[3-(13-hydroxy-2-oxoazacyclohexadec-1-yl)propyl]- (9CI) (CA INDEX NAME)

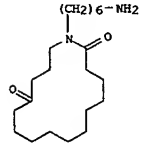
L4 ANSWER 10 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



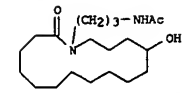
RN 152450-30-1 CAPLUS
CN Azacyclohexadecane-2,13-dione, 1-(4-aminobutyl)- (9CI) (CA INDEX NAME)



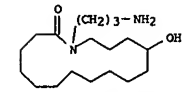
RN 152450-31-2 CAPLUS
CN Azacyclohexadecane-2,13-dione, 1-(6-aminohexyl)- (9CI) (CA INDEX NAME)



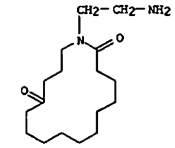
L4 ANSWER 10 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



RN 152450-35-6 CAPLUS
CN Azacyclohexadecan-2-one, 1-(3-aminopropyl)-13-hydroxy- (9CI) (CA INDEX NAME)

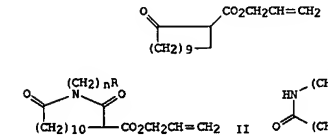


IT **152450-27-6P 152450-28-7P 152450-30-1P 152450-31-2P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and mass spectrum of, water loss in)
RN 152450-27-6 CAPLUS
CN Azacyclohexadecane-2,13-dione, 1-(2-aminoethyl)- (9CI) (CA INDEX NAME)

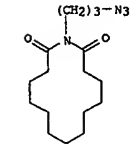


RN 152450-28-7 CAPLUS
CN Azacyclohexadecane-2,13-dione, 1-(3-aminopropyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 11 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1992:174126 CAPLUS
DOCUMENT NUMBER: 116:174126
TITLE: Synthesis of macrocycles by ring enlargement of 14-membered cyclic imides
AUTHOR(S): Koch, Thomas; Ognyanov, Vassil I.; Hesse, Manfred
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, CH-8057, Switz.
SOURCE: Helvetica Chimica Acta (1992), 75(1), 62-8
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 116:174126
GI

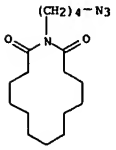


AB In the presence of a base, cyclododecanone deriv. I, activated in .alpha.-position by the allyloxycarbonyl group, underwent ring enlargement with isocyanates to give 14-membered imides II (n = 3, R = Cl; n = 4, R = Br). Cleavage of the activating group gave new 14-membered imides which were transformed by further ring-enlargement reactions into the new macrocyclic compds. III.
IT **139662-47-8P 139662-48-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and transamidation of)
RN 139662-47-8 CAPLUS
CN Azacyclotetradecane-2,14-dione, 1-(3-azidopropyl)- (9CI) (CA INDEX NAME)



RN 139662-48-9 CAPLUS
CN Azacyclotetradecane-2,14-dione, 1-(4-azidobutyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 11 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



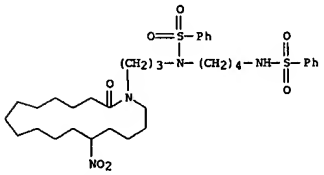
L4 ANSWER 12 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1989:554188 CAPLUS
DOCUMENT NUMBER: 111:154188
TITLE: Syntheses of the spermidine alkaloids (.+-.)-inandenin-10-ol, inandenin-10-one, and (.+-.)-oncinotine
AUTHOR(S): Bienz, Stefan; Guggisberg, Armin; Waelchli, Rudolf; Hesse, Manfred
CORPORATE SOURCE: Org. Chem. Inst., Univ. Zurich, Zurich, CH-8057, Switz.
SOURCE: Helvetica Chimica Acta (1988), 71(7), 1708-18
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 111:154188
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

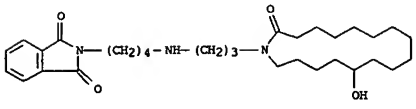
AB (.+-.)-Inandenin-10-ol (I, X = H,HO), inandenin-10-one (I, X = O) and (.+-.)-oncinotine (II) were prepd. from the aldehyde III and PhSO2NH(CH2)4N(SO2Ph)(CH2)3NH2 via ring expansion of the dodecanone deriv. IV and transamidation of the lactam V.

IT **122890-18-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and Neff reaction of)
RN 122890-18-0 CAPLUS
CN Benzenesulfonamide, N-[3-(13-nitro-2-oxoazacycloheptadec-1-yl)propyl]-N-[4-[(phenylsulfonyl)amino]butyl]- (9CI) (CA INDEX NAME)



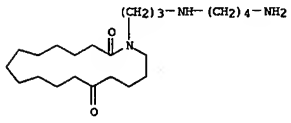
IT **122890-28-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and chlorination of)
RN 122890-28-2 CAPLUS
CN 1H-Isoindole-1,3(2H)-dione, 2-[4-[[3-(13-hydroxy-2-oxoazacycloheptadec-1-yl)propyl]amino]butyl]-, monohydrochloride (9CI) (CA INDEX NAME)

L4 ANSWER 12 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



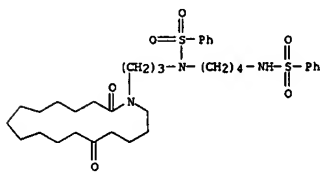
● HCl

IT **122890-26-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conversion to phthalimido deriv.)
RN 122890-26-0 CAPLUS
CN Azacycloheptadecane-2,13-dione, 1-[3-[(4-aminobutyl)amino]propyl]-, dihydrochloride (9CI) (CA INDEX NAME)



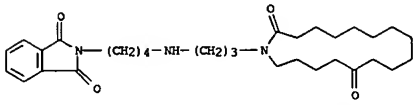
●2 HCl

IT **122890-19-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and electrochem. redn. of)
RN 122890-19-1 CAPLUS
CN Benzenesulfonamide, N-[3-(2,13-dioxoazacycloheptadec-1-yl)propyl]-N-[4-[(phenylsulfonyl)amino]butyl]- (9CI) (CA INDEX NAME)

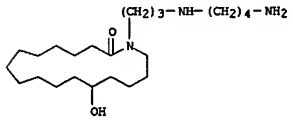


L4 ANSWER 12 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

IT **122890-27-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and intramol. cyclization of)
RN 122890-27-1 CAPLUS
CN Azacycloheptadecane-2,13-dione, 1-[3-[[4-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)butyl]amino]propyl]- (9CI) (CA INDEX NAME)

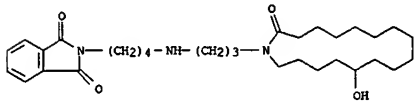


IT **122890-20-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and ring expansion of)
RN 122890-20-4 CAPLUS
CN Azacycloheptadecan-2-one, 1-[3-[(4-aminobutyl)amino]propyl]-13-hydroxy-, dihydrochloride (9CI) (CA INDEX NAME)

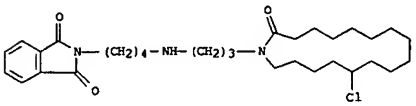


●2 HCl

IT **122890-23-7P 122890-24-8P 122890-29-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 122890-23-7 CAPLUS
CN 1H-Isoindole-1,3(2H)-dione, 2-[4-[[3-(13-hydroxy-2-oxoazacycloheptadec-1-yl)propyl]amino]butyl]- (9CI) (CA INDEX NAME)

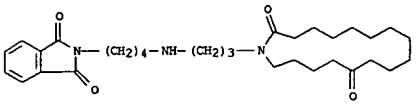


L4 ANSWER 12 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
RN 122890-24-8 CAPLUS
CN 1H-Isoindole-1,3(2H)-dione, 2-[4-[[3-(13-chloro-2-oxoazacycloheptadec-1-yl)propyl]amino]butyl]-, monohydrochloride (9CI) (CA INDEX NAME)



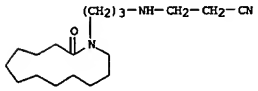
● HCl

RN 122890-29-3 CAPLUS
CN Azacycloheptadecane-2,13-dione, 1-[3-[[4-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)butyl]amino]propyl]-, dihydrochloride (9CI) (CA INDEX NAME)



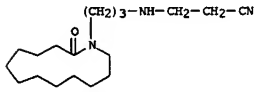
●2 HCl

L4 ANSWER 13 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

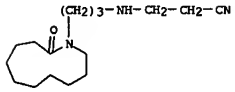


● HCl

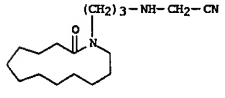
IT 67171-82-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, in presence of strong base)
RN 67171-82-8 CAPLUS
CN Propanenitrile, 3-[[3-(2-oxoazacyclotridec-1-yl)propyl]amino]- (9CI) (CA INDEX NAME)



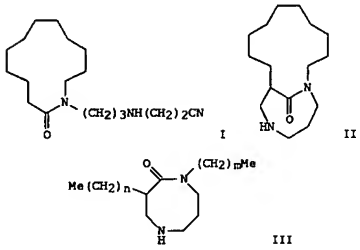
IT 99014-88-7P 99014-95-6P 99014-96-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and cyclization of)
RN 99014-88-7 CAPLUS
CN Propanenitrile, 3-[[3-(2-oxoazacycloundec-1-yl)propyl]amino]- (9CI) (CA INDEX NAME)



RN 99014-95-6 CAPLUS
CN Acetonitrile, [[3-(2-oxoazacyclotridec-1-yl)propyl]amino]- (9CI) (CA INDEX NAME)

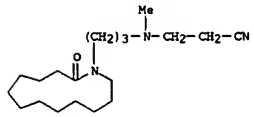


L4 ANSWER 13 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1986:5757 CAPLUS
DOCUMENT NUMBER: 104:5757
TITLE: Transamidation reactions. Part 11. N-Substituted 3-aminopropanenitriles and 2-aminoacetonitriles as Schiff-base equivalents
AUTHOR(S): Askitoglu, Elefteria; Guggisberg, Armin; Hesse, Manfred
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, CH-8057, Switz.
SOURCE: Helvetica Chimica Acta (1985), 68(3), 750-9
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 104:5757
GI

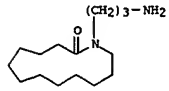


AB Treating (oxoazacyclotridecyl)azaheptanenitrile I with KNH(CH2)3NH2-NH2(CH2)3NH2 or with Me3COK-PhMe gave the unexpected bicyclic product II. Similarly, treatment of Me(CH2)nCH2CON[(CH2)mMe](CH2)3NH(CH2)6CN (n = m = 0; n = 4, m = 5) with Me3COK-PhMe gave the diazacyclooctanones III. The reaction proceeds via an intermediate formaldehyde imine.
IT 99014-99-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of)
RN 99014-99-0 CAPLUS
CN Propanenitrile, 3-[[3-(2-oxoazacyclotridec-1-yl)propyl]amino]-, monohydrochloride (9CI) (CA INDEX NAME)

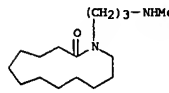
L4 ANSWER 13 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
RN 99014-96-7 CAPLUS
CN Propanenitrile, 3-[methyl[3-(2-oxoazacyclotridec-1-yl)propyl]amino]- (9CI) (CA INDEX NAME)



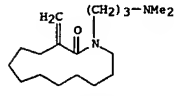
IT 64414-61-5P 67370-86-9P 99014-86-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 64414-61-5 CAPLUS
CN Azacyclotridecan-2-one, 1-(3-aminopropyl)- (9CI) (CA INDEX NAME)



RN 67370-86-9 CAPLUS
CN Azacyclotridecan-2-one, 1-[3-(methylamino)propyl]- (9CI) (CA INDEX NAME)

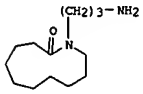


RN 99014-86-5 CAPLUS
CN Azacyclotridecan-2-one, 1-[3-(dimethylamino)propyl]-3-methylene- (9CI) (CA INDEX NAME)

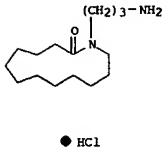


IT 67370-80-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with acrylonitrile)
RN 67370-80-3 CAPLUS

L4 ANSWER 13 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
CN Azacycloundecan-2-one, 1-(3-aminopropyl)- (9CI) (CA INDEX NAME)

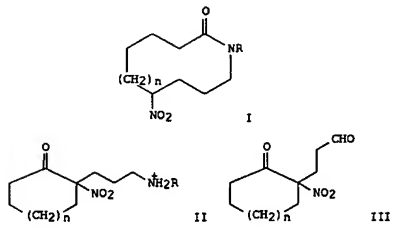


IT 99014-94-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactions of)
RN 99014-94-5 CAPLUS
CN Azacyclotridecan-2-one, 1-(3-aminopropyl)-, monohydrochloride (9CI) (CA INDEX NAME)



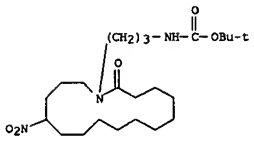
● HCl

L4 ANSWER 14 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1986:5756 CAPLUS
DOCUMENT NUMBER: 104:5756
TITLE: Synthesis of macrocyclic lactams from ketones by ring enlargement reaction
AUTHOR(S): Waelchli, Rudolf; Bienz, Stefan; Hesse, Manfred
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, CH-8057, Switz.
SOURCE: Helvetica Chimica Acta (1985), 68(2), 484-92
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 104:5756
GI



AB The macrocyclic lactams I [R = PhCH2, n = 1, 3, 7; R = Pr, n = 3, 7; R = Me(CH2)4, Me3C, HO(CH2)3, Me3CO2CNH(CH2)3, n = 7] were prepd. by ring expansion of the (aminopropyl)nitrocycloalkanones II by treatment with NaHCO3 in H2O/MeOH. II were prepd. by reductive amination of the aldehydes III.
IT 99379-76-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 99379-76-7 CAPLUS
CN Carbamic acid, [3-(13-nitro-2-oxoazacyclohexadec-1-yl)propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

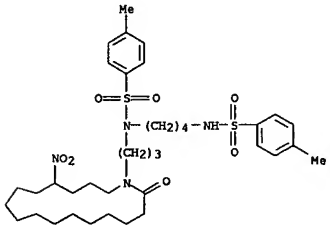
L4 ANSWER 14 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



L4 ANSWER 15 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1985:221067 CAPLUS
DOCUMENT NUMBER: 102:221067
TITLE: Synthesis of N-(4-aminobutyl)-16-aza-19-nonadecane lactam and N-(4-aminobutyl)-17-aza-20-icosane lactam (deoxoinandenine)
AUTHOR(S): Waelchli, Rudolf; Guggisberg, Armin; Hesse, Manfred
CORPORATE SOURCE: Org. Chem. Inst., Univ. Zurich, Zurich, CH-8057, Switz.
SOURCE: Helvetica Chimica Acta (1984), 67(8), 2178-85
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
GI

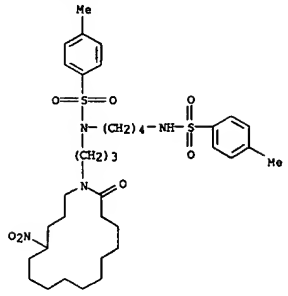
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I (n = 1, 0) were prepd. from cyclotridecanone and cyclododecanone, resp. via ring enlargement of the aminopropyl cycloalkanone derivs. II and III.
IT 91653-21-3P 96624-95-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conversion to ketone)
RN 91653-21-3 CAPLUS
CN Benzenesulfonamide, 4-methyl-N-[4-[[(4-methylphenyl)sulfonyl]amino]butyl]-N-[3-(14-nitro-2-oxoazacycloheptadec-1-yl)propyl]- (9CI) (CA INDEX NAME)

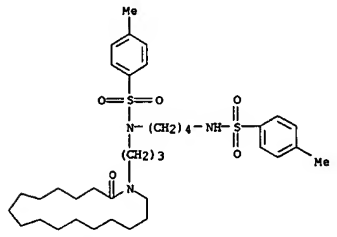


RN 96624-95-2 CAPLUS
CN Benzenesulfonamide, 4-methyl-N-[4-[[(4-methylphenyl)sulfonyl]amino]butyl]-N-[3-(13-nitro-2-oxoazacyclohexadec-1-yl)propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

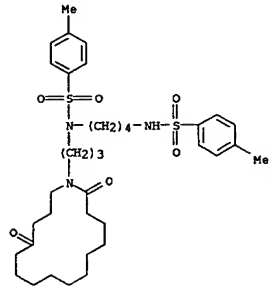


IT **91652-54-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and detolsylation of)
RN 91652-54-9 CAPLUS
CN Benzenesulfonamide, 4-methyl-N-[4-[[(4-methylphenyl)sulfonyl]amino]butyl]-N-[3-(2-oxoazacycloheptadec-1-yl)propyl]- (9CI) (CA INDEX NAME)

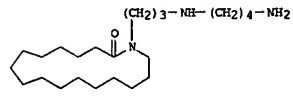


IT **96624-97-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and detosylation of)
RN 96624-97-4 CAPLUS
CN Benzenesulfonamide, 4-methyl-N-[4-[[(4-methylphenyl)sulfonyl]amino]butyl]-

L4 ANSWER 15 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
CN Benzenesulfonamide, N-[3-(2,13-dioxoazacyclohexadec-1-yl)propyl]-4-methyl-N-[4-[[(4-methylphenyl)sulfonyl]amino]butyl]- (9CI) (CA INDEX NAME)

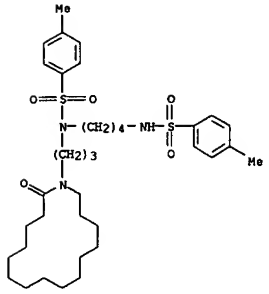


IT **91653-20-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and ring enlargement of, (aminobutyl)azaicosane lactam from)
RN 91653-20-2 CAPLUS
CN Azacycloheptadecan-2-one, 1-[3-[(4-aminobutyl)amino]propyl]- (9CI) (CA INDEX NAME)

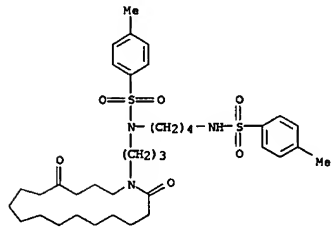


IT **96624-94-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and ring enlargement of, (aminobutyl)azanondecane lactam from)
RN 96624-94-1 CAPLUS
CN Azacyclohexadecan-2-one, 1-[3-[(4-aminobutyl)amino]propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
N-[3-(2-oxoazacyclohexadec-1-yl)propyl]- (9CI) (CA INDEX NAME)

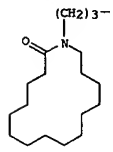


IT **91652-53-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and ketalization of ethylenedithiol)
RN 91652-53-8 CAPLUS
CN Benzenesulfonamide, N-[3-(2,14-dioxoazacycloheptadec-1-yl)propyl]-4-methyl-N-[4-[[(4-methylphenyl)sulfonyl]amino]butyl]- (9CI) (CA INDEX NAME)

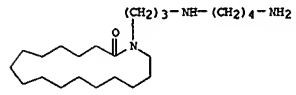


IT **96624-96-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and ketalization with ethanedithiol)
RN 96624-96-3 CAPLUS

L4 ANSWER 15 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

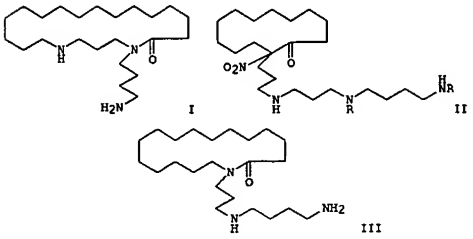


IT **96624-98-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 96624-98-5 CAPLUS
CN Azacycloheptadecan-2-one, 1-[3-[(4-aminobutyl)amino]propyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

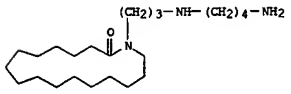
L4 ANSWER 16 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1984:511239 CAPLUS
DOCUMENT NUMBER: 101:111239
TITLE: Ring expansion reactions in the formation of macrocyclic lactams. A synthesis of deoxoinandenine
AUTHOR(S): Waelchli, Rudolf; Guggisberg, Armin; Hesse, Manfred
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zuerich, Zurich, CH-8057, Switz.
SOURCE: Tetrahedron Letters (1984), 25(21), 2205-8
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Deoxoinandenine (I), a redn. product of the macrocyclic spermidine alkaloids inandenin-12-one and -13-one was synthesized starting from 2-nitrocyclotridecanone by ring expansion reactions of macrocycles II (R = p-MeC6H4SO2) and III.

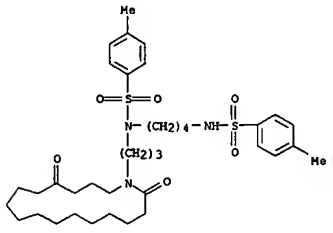
IT **91653-20-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and Zip ring expansion of)

RN 91653-20-2 CAPLUS
CN Azacycloheptadecan-2-one, 1-[3-[(4-aminobutyl)amino]propyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 16 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and redn. of)

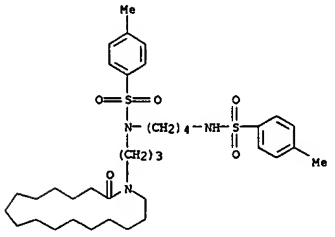
RN 91652-53-8 CAPLUS
CN Benzenesulfonamide, N-[3-(2,14-dioxoazacycloheptadec-1-yl)propyl]-4-methyl-N-[4-[[(4-methylphenyl)sulfonyl]amino]butyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 16 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

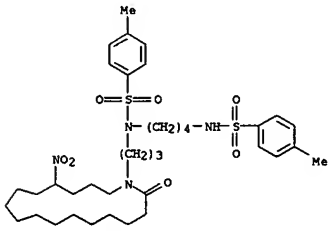
IT **91652-54-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and detosylation of)

RN 91652-54-9 CAPLUS
CN Benzenesulfonamide, 4-methyl-N-[4-[[(4-methylphenyl)sulfonyl]amino]butyl]-N-[3-(2-oxoazacycloheptadec-1-yl)propyl]- (9CI) (CA INDEX NAME)



IT **91653-21-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and hydrolysis of)

RN 91653-21-3 CAPLUS
CN Benzenesulfonamide, 4-methyl-N-[4-[[(4-methylphenyl)sulfonyl]amino]butyl]-N-[3-(14-nitro-2-oxoazacycloheptadec-1-yl)propyl]- (9CI) (CA INDEX NAME)

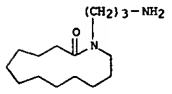


IT **91652-53-8P**

L4 ANSWER 17 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1981:496437 CAPLUS
DOCUMENT NUMBER: 95:96437
TITLE: Transamidation reactions. Part 9. Amidines as intermediates in transamidation reactions
AUTHOR(S): Heidelberger, Christian; Guggisberg, Armin; Stephanou, Euripides; Hesse, Manfred
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, CH-8057, Switz.
SOURCE: Helvetica Chimica Acta (1981), 64(2), 399-406
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB Refluxing N-(aminoalkyl) lactams in xylene contg. p-MeC6H4SO3H gave bicyclic amidines, which were partially hydrolyzed in aq. KOH to give the starting and a ring-enlarged lactam. An example was the conversion of I to II, followed by hydrolysis to give I and III. N-[(Alkylamino)alkyl] lactams follow an analogous course via amidinium salts; e.g., IV was converted to V, which was hydrolyzed to give IV and VI. In some cases only 1 of the 2 isomeric lactams was formed in the alk. hydrolysis step.

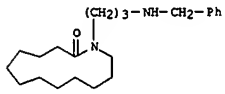
IT **64414-61-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, amidine formation in)

RN 64414-61-5 CAPLUS
CN Azacyclotridecan-2-one, 1-(3-aminopropyl)- (9CI) (CA INDEX NAME)



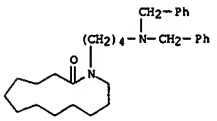
IT **72636-84-1 78097-27-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(ring enlargement of, in transamidation)

RN 72636-84-1 CAPLUS
CN Azacyclotridecan-2-one, 1-[3-[(phenylmethyl)amino]propyl]- (9CI) (CA INDEX NAME)



RN 78097-27-5 CAPLUS
CN Azacyclotridecan-2-one, 1-[4-[bis(phenylmethyl)amino]butyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 17 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



L4 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1980:128882 CAPLUS
DOCUMENT NUMBER: 92:128882
TITLE: Transamidation reactions. Part 8. Use of the 'Zip' reaction for the synthesis of a 53-membered polyamino lactam
AUTHOR(S): Kramer, Urs; Guggisberg, Armin; Hesse, Manfred
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, CH-8057, Switz.
SOURCE: Helvetica Chimica Acta (1979), 62(7), 2317-24
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The lactam I reacted with K 3-aminopropylamide/1,3-diaminopropane (Zip reaction) to give the 53-membered lactam II. I was prepd. in 8 steps from III and PhNH[(CH2)2N(TOS)]3(CH2)3I (TOS = tosyl).

IT 73100-38-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and benzylation of)

RN 73100-38-6 CAPLUS

CN Benzenesulfonamide, N-[19-amino-4,8,12,16-tetrakis[(4-methylphenyl)sulfonyl]-4,8,12,16-tetraazanonadec-1-yl]-4-methyl-N-[4,8,12,16-tetrakis[(4-methylphenyl)sulfonyl]-19-(2-oxoazacyclotridec-1-yl)-4,8,12,16-tetraazanonadec-1-yl]-, monohydrochloride (9CI) (CA INDEX NAME)

L4 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

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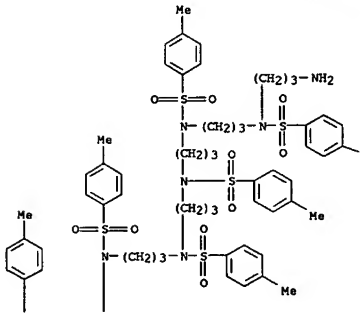

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L4 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

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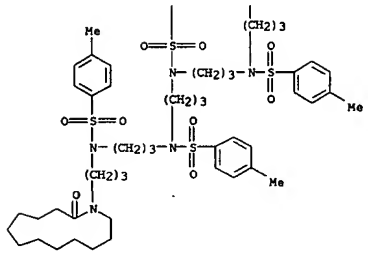

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● HCl

IT 65605-32-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and chain lengthening of)

RN 65605-32-5 CAPLUS

CN Benzenesulfonamide, 4-methyl-N-[3-[[(4-methylphenyl)sulfonyl][3-[[(4-methylphenyl)sulfonyl]amino]propyl]amino]propyl]-N-[3-[[(4-methylphenyl)sulfonyl][3-[[(4-methylphenyl)sulfonyl][3-[[(4-methylphenyl)sulfonyl][3-[(2-oxoazacyclotridec-1-yl)amino]propyl]amino]propyl]amino]propyl]amino]propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

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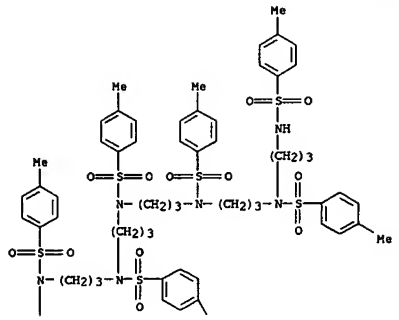

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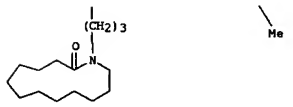

IT 65605-33-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and electrolysis of)
RN 65605-33-6 CAPLUS
CN Benzenesulfonamide, 4-methyl-N-[4,8,12,16-tetrakis[(4-methylphenyl)sulfonyl]-19-(2-oxoazacyclotridec-1-yl)-4,8,12,16-tetraazanonadec-1-yl]-N-[4,8,12,16-tetrakis[(4-methylphenyl)sulfonyl]-21-phenyl-20-(phenylmethyl)-4,8,12,16,20-pentaazaheneicos-1-yl]- (9CI) (CA INDEX NAME)

L4 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

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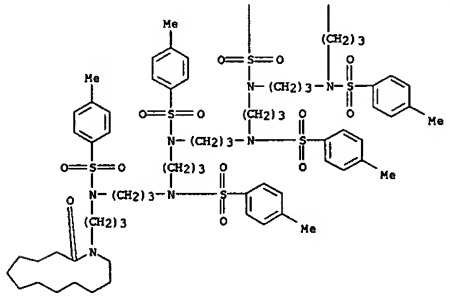

IT 73100-39-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and hydrogenolysis of)
RN 73100-39-7 CAPLUS
CN Azacyclotridecan-2-one, 1-[41-phenyl-40-(phenylmethyl)-4,8,12,16,20,24,28,32,36-nonaazahentetracont-1-yl]- (9CI) (CA INDEX NAME)

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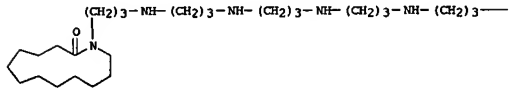

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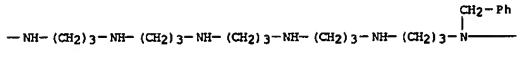

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L4 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

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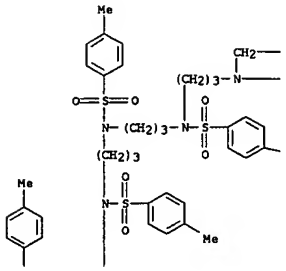

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L4 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

IT 73100-35-3P 73100-37-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with hydrazine)
RN 73100-35-3 CAPLUS
CN Benzenesulfonamide, N-[3-[[3-[[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propyl][(4-methylphenyl)sulfonyl]amino]propyl][(4-methylphenyl)sulfonyl]amino]propyl]-4-methyl-N-[3-[[(4-methylphenyl)sulfonyl][3-[[(4-methylphenyl)sulfonyl][3-(2-oxoazacyclotridec-1-yl)propyl]amino]propyl]amino]propyl]- (9CI) (CA INDEX NAME)

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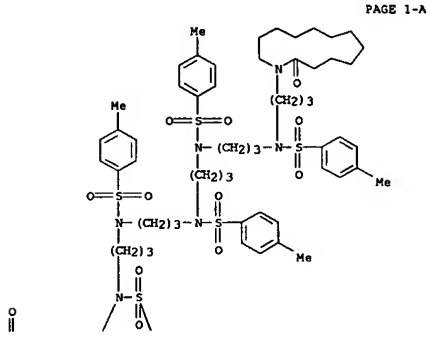

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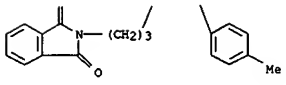

RN 73100-37-5 CAPLUS
CN Benzenesulfonamide, N-[19-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)-4,8,12,16-tetrakis[(4-methylphenyl)sulfonyl]-4,8,12,16-tetraazanonadec-1-yl]-4-methyl-N-[4,8,12,16-tetrakis[(4-methylphenyl)sulfonyl]-19-(2-oxoazacyclotridec-1-yl)-4,8,12,16-tetraazanonadec-1-yl]- (9CI) (CA INDEX NAME)

L4 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

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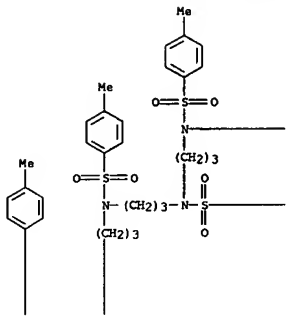

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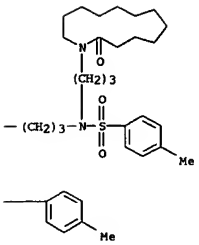

L4 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

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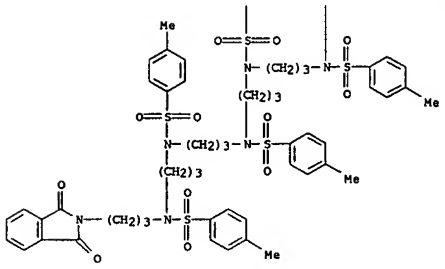

IT 65605-34-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and ring expansion of)
RN 65605-34-7 CAPLUS
CN Azacyclotridecan-2-one, 1-(39-amino-4,8,12,16,20,24,28,32,36-nonaazanonatriacont-1-yl)- (9CI) (CA INDEX NAME)

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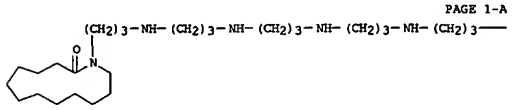

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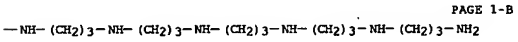

IT 73100-36-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and tosylation of)
RN 73100-36-4 CAPLUS
CN Benzenesulfonamide, N-[3-[[3-[(3-aminopropyl)[(4-methylphenyl)sulfonyl]amino]propyl][(4-methylphenyl)sulfonyl]amino]propyl]-4-methyl-N-[3-[[(4-methylphenyl)sulfonyl][3-[[(4-methylphenyl)sulfonyl][3-

L4 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
(2-oxoazacyclotridec-1-yl)propyl]amino]propyl]amino]propyl]- (9CI) (CA INDEX NAME)

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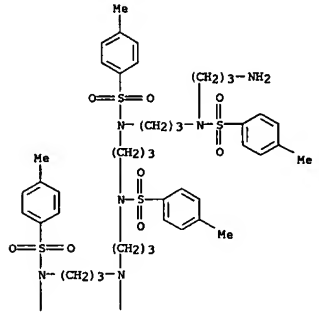

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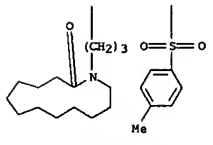

IT 73100-41-1P 73100-42-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 73100-41-1 CAPLUS
CN Azacyclotridecan-2-one, 1-[41-phenyl-40-(phenylmethyl)-4,8,12,16,20,24,28,32,36-nonaazahentetracont-1-yl)-, decahydrochloride (9CI) (CA INDEX NAME)

L4 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

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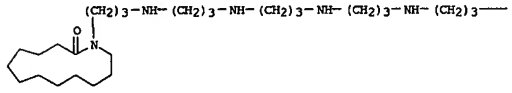

●10 HCl

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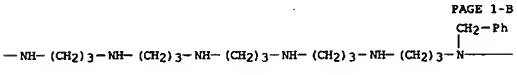

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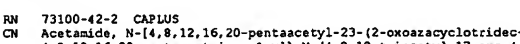

RN 73100-42-2 CAPLUS
CN Acetamide, N-[4,8,12,16,20-pentaacetyl-23-(2-oxoazacyclotridec-1-yl)-4,8,12,16,20-pentaazatricos-1-yl]-N-(4,8,12-triacetyl-17-oxo-4,8,12,16-tetraazaoctadec-1-yl)- (9CI) (CA INDEX NAME)

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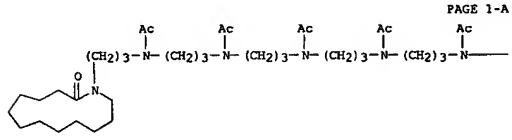

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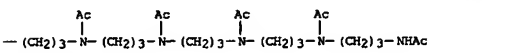
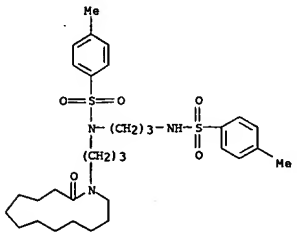
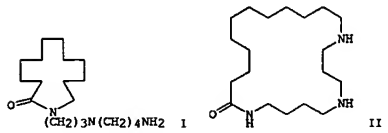


IT 65545-59-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with iodopropyltripropylenetetramine deriv.)
RN 65545-59-7 CAPLUS

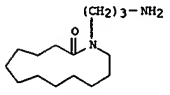
L4 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
CN Benzenesulfonamide, 4-methyl-N-[3-[[(4-methylphenyl)sulfonyl]amino]propyl]-N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 19 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1980:93862 CAPLUS
DOCUMENT NUMBER: 92:93862
TITLE: Transamidation reactions. Part 7. Ring enlargement reactions of N-(2-aminoethyl), N-(4-aminobutyl), N-(6-amino-4-azahexyl), and N-(8-amino-4-azaoctyl) lactams
AUTHOR(S): Stephanou, Euripides; Guggisberg, Armin; Hesse, Manfred
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, CH-8057, Switz.
SOURCE: Helvetica Chimica Acta (1979), 62(6), 1932-43
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
GI

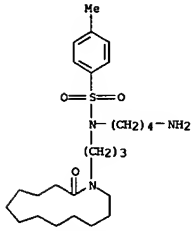


AB Five N-(aminoalkyl) lactams, with 7-, 8-, 9- and 13-membered rings, e.g., I, were prepd. and treated with XNH(CH2)3NH2 in H2N(CH2)3NH2. The caprolactam was stable and did not react, but the others rearranged with ring enlargement; e.g., I rearranged rapidly to a 17-membered ring and, after a longer period, to the 22-membered ring II and H2N(CH2)3NHCO(CH2)11NH(CH2)3NH(CH2)4NH2. The results show that the 7-membered lactam ring was more stable than the 10-membered ring to which it did not rearrange, but the 8-membered lactam ring was less stable than the 11-membered ring to which it did rearrange.
IT **64414-61-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with benzaldehyde followed by redn.)
RN 64414-61-5 CAPLUS
CN Azacyclotridecan-2-one, 1-(3-aminopropyl)- (9CI) (CA INDEX NAME)

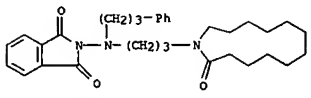


IT **72636-91-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

L4 ANSWER 19 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
(Reactant or reagent)
(prepn. and detosylation of)
RN 72636-91-0 CAPLUS
CN Benzenesulfonamide, N-(4-aminobutyl)-4-methyl-N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

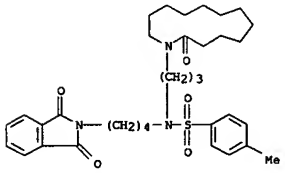


IT **72636-85-2P 72636-90-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and hydrazinolysis of)
RN 72636-85-2 CAPLUS
CN 1H-Isoindole-1,3(2H)-dione, 2-[[3-(2-oxoazacyclotridec-1-yl)propyl](3-phenylpropyl)amino]- (9CI) (CA INDEX NAME)

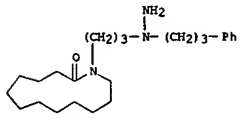


RN 72636-90-9 CAPLUS
CN Benzenesulfonamide, N-[4-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)butyl]-4-methyl-N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

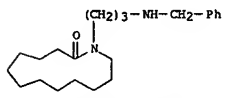
L4 ANSWER 19 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



IT **72636-86-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and hydrogenolysis of)
RN 72636-86-3 CAPLUS
CN Azacyclotridecan-2-one, 1-[3-[1-(3-phenylpropyl)hydrazino]propyl]- (9CI) (CA INDEX NAME)

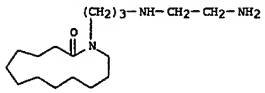


IT **72636-84-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and phthalimido ethylation of)
RN 72636-84-1 CAPLUS
CN Azacyclotridecan-2-one, 1-[3-[(phenylmethyl)amino]propyl]- (9CI) (CA INDEX NAME)

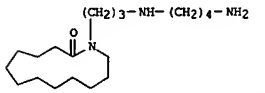


IT **72636-88-5P 72636-92-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and ring enlargement reaction of)
RN 72636-88-5 CAPLUS
CN Azacyclotridecan-2-one, 1-[3-[(2-aminoethyl)amino]propyl]- (9CI) (CA INDEX NAME)

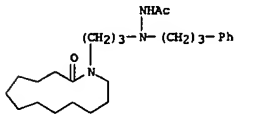
L4 ANSWER 19 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



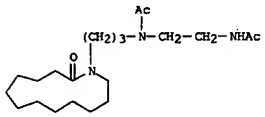
RN 72636-92-1 CAPLUS
CN Azacyclotridecan-2-one, 1-[3-[(4-aminobutyl)amino]propyl]- (9CI) (CA INDEX NAME)



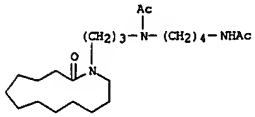
IT **72636-87-4P 72636-89-6P 72636-93-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 72636-87-4 CAPLUS
CN Acetic acid, 2-[3-(2-oxoazacyclotridec-1-yl)propyl]-2-(3-phenylpropyl)hydrazide (9CI) (CA INDEX NAME)



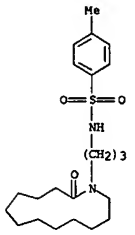
RN 72636-89-6 CAPLUS
CN Acetamide, N-[2-(acetylamino)ethyl]-N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



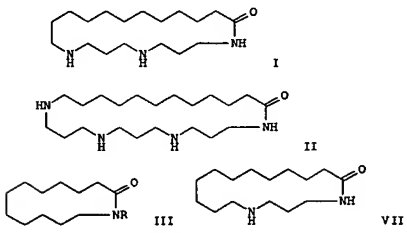
L4 ANSWER 19 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
RN 72636-93-2 CAPLUS
CN Acetamide, N-[4-(acetylamino)butyl]-N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



IT **67370-84-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with (bromobutyl)phthalamide)
RN 67370-84-7 CAPLUS
CN Benzenesulfonamide, 4-methyl-N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



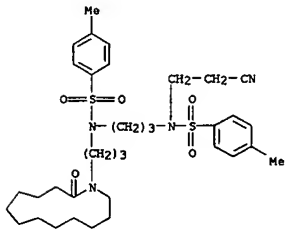
L4 ANSWER 20 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1978:509418 CAPLUS
DOCUMENT NUMBER: 89:109418
TITLE: The Zip reaction: a new ring expansion reaction. Synthesis of 17-, 21- and 25-membered polyaminolactams
AUTHOR(S): Kramer, Urs; Guggisberg, Armin; Hesse, Manfred; Schmid, Hans
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, Switz.
SOURCE: Helvetica Chimica Acta (1978), 61(4), 1342-52
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



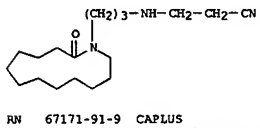
AB The 21- and 25-membered aminolactams I and II were prepd. by introducing the ring enlargement unit (aminopropyl group) into III (R = H), followed by conversion into the heterocyclic lactam by strong base. N-alkylation of III (R = H) with H2C:CHCN, followed by hydrogenation gave III [R = (CH2)3NH2] (IV), and repetition of this process once and twice gave III [R = (CH2)3NH(CH2)3NH2] (V) and III [R = (CH2)3NH(CH2)3NH(CH2)3NH2] (VI). Treatment of IV, V, and VI with base (zip reaction) gave the lactams VII, I and II, resp. I was also obtained stepwise by aminopropylation and ring enlargement of VII.

IT **67171-90-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and deblocking of)
RN 67171-90-8 CAPLUS
CN Benzenesulfonamide, N-(2-cyanoethyl)-4-methyl-N-[3-[[(4-methylphenyl)sulfonyl][3-(2-oxoazacyclotridec-1-yl)propyl]amino]propyl]- (9CI) (CA INDEX NAME)

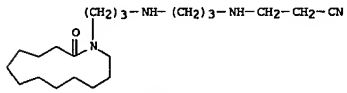
L4 ANSWER 20 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



IT **67171-82-8P 67171-91-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and redn. of)
RN 67171-82-8 CAPLUS
CN Propanenitrile, 3-[[3-(2-oxoazacyclotridec-1-yl)propyl]amino]- (9CI) (CA INDEX NAME)

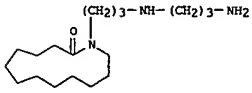


RN 67171-91-9 CAPLUS
CN Propanenitrile, 3-[[3-[[3-(2-oxoazacyclotridec-1-yl)propyl]amino]propyl]amino]- (9CI) (CA INDEX NAME)

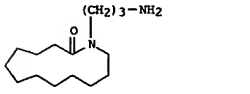


IT **64414-60-4P 64414-61-5P 67473-75-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and ring expansion of)
RN 64414-60-4 CAPLUS
CN Azacyclotridecan-2-one, 1-[3-[(3-aminopropyl)amino]propyl]- (9CI) (CA INDEX NAME)

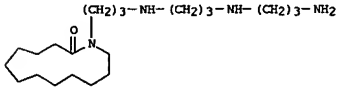
L4 ANSWER 20 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



RN 64414-61-5 CAPLUS
CN Azacyclotridecan-2-one, 1-(3-aminopropyl)- (9CI) (CA INDEX NAME)

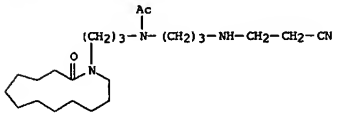


RN 67473-75-0 CAPLUS
CN Azacyclotridecan-2-one, 1-[3-[[3-[(3-aminopropyl)amino]propyl]amino]propyl]- (9CI) (CA INDEX NAME)

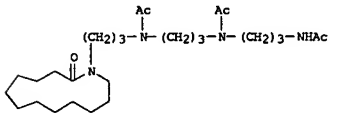


IT 65545-59-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and N-alkylation of, by acrylonitrile)
RN 65545-59-7 CAPLUS
CN Benzenesulfonamide, 4-methyl-N-[3-[[(4-methylphenyl)sulfonyl]amino]propyl]-N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

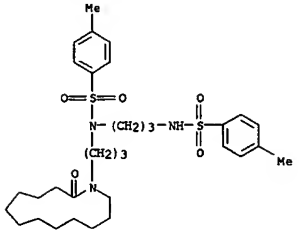
L4 ANSWER 20 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



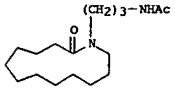
RN 67473-76-1 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-[acetyl[3-(2-oxoazacyclotridec-1-yl)propyl]amino]propyl]- (9CI) (CA INDEX NAME)



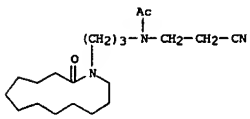
L4 ANSWER 20 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



IT 67171-81-7P 67171-83-9P 67171-92-0P
67473-76-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 67171-81-7 CAPLUS
CN Acetamide, N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

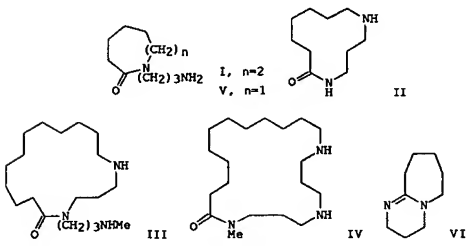


RN 67171-83-9 CAPLUS
CN Acetamide, N-(2-cyanoethyl)-N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



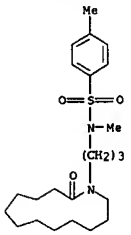
RN 67171-92-0 CAPLUS
CN Acetamide, N-[3-[(2-cyanoethyl)amino]propyl]-N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 21 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1978:509412 CAPLUS
DOCUMENT NUMBER: 89:109412
TITLE: Transamidation reactions of cyclic amino amides
AUTHOR(S): Guggisberg, Armin; Kramer, Urs; Heidelberger, Christian; Charubala, Ramamurty; Stephanou, Euripides; Hesse, Manfred; Schmid, Hans
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, Switz.
SOURCE: Helvetica Chimica Acta (1978), 61(3), 1050-63
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
GI

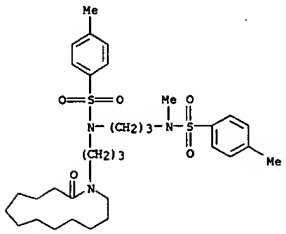


AB Lactams which are substituted at the N atom by a 3-aminopropyl residue were transformed under base catalysis to a cyclic amide enlarged by 4 ring atoms. The formed rings must have a min. of 12 members. Thus, the lactam I was transamidated in 96% yield to give the 12-membered ring II in the presence of H2NCH2CH2CONH2.K in H2N(CH2)3NH2. Large ring lactams which are substituted at the N by a 3-(alkylamino)propyl group lead under base catalysis to an equil. mixt., e.g. the 17-membered lactam III was in equil. with the 21-membered amino amide IV. Transamidation of the lactam V didn't give the expected amino amide, but gave the water elimination product VI.
IT 67370-85-8P 67370-88-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and detosylation of)
RN 67370-85-8 CAPLUS
CN Benzenesulfonamide, N,4-dimethyl-N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 21 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

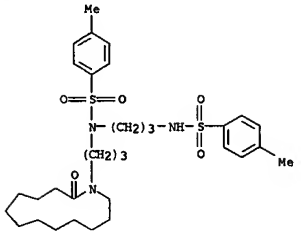


RN 67370-88-1 CAPLUS
CN Benzenesulfonamide, N,4-dimethyl-N-[3-[[(4-methylphenyl)sulfonyl][3-(2-oxoazacyclotridec-1-yl)propyl]amino]propyl]- (9CI) (CA INDEX NAME)

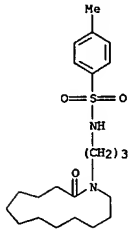


IT **65545-59-7P 67370-84-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and methylation of)
RN 65545-59-7 CAPLUS
CN Benzenesulfonamide, 4-methyl-N-[3-[[(4-methylphenyl)sulfonyl]amino]propyl]-N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 21 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

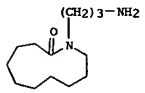


RN 67370-84-7 CAPLUS
CN Benzenesulfonamide, 4-methyl-N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

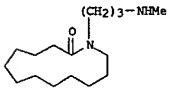


IT **67370-80-3P 67370-86-9P 67370-89-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and transamidation of)
RN 67370-80-3 CAPLUS
CN Azacycloundecan-2-one, 1-(3-aminopropyl)- (9CI) (CA INDEX NAME)

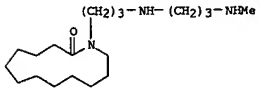
L4 ANSWER 21 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



RN 67370-86-9 CAPLUS
CN Azacyclotridecan-2-one, 1-[3-(methylamino)propyl]- (9CI) (CA INDEX NAME)

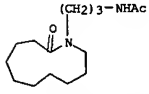


RN 67370-89-2 CAPLUS
CN Azacyclotridecan-2-one, 1-[3-[[3-(methylamino)propyl]amino]propyl]-, dihydrochloride (9CI) (CA INDEX NAME)



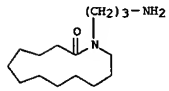
●2 HCl

IT **67370-81-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 67370-81-4 CAPLUS
CN Acetamide, N-[3-(2-oxoazacycloundec-1-yl)propyl]- (9CI) (CA INDEX NAME)

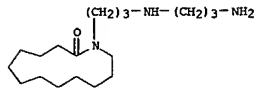


IT **64414-61-5 67370-92-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with toluenesulfonyl chloride)
RN 64414-61-5 CAPLUS
CN Azacyclotridecan-2-one, 1-(3-aminopropyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 21 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

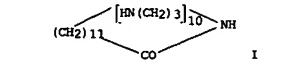


RN 67370-92-7 CAPLUS
CN Azacyclotridecan-2-one, 1-[3-[(3-aminopropyl)amino]propyl]-, hydrochloride (9CI) (CA INDEX NAME)

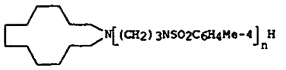


●x HCl

L4 ANSWER 22 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1978:136588 CAPLUS
DOCUMENT NUMBER: 88:136588
TITLE: Transamidation reactions. 5. Application of the "zip" reaction to the synthesis of a 53-membered polyaminolactam
AUTHOR(S): Kramer, Urs; Guggisberg, Armin; Hesse, Manfred; Schmid, Hans
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, Switz.
SOURCE: Angewandte Chemie (1978), 90(3), 210-11
CODEN: ANCEAD; ISSN: 0044-8249
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



I



II

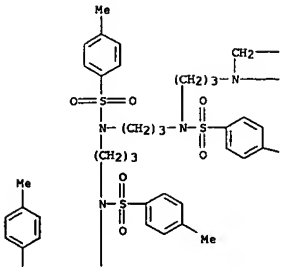
AB The macrocycle I was prepd. from N-(3-brompropyl)phthalimide and tosylhydrazine via II (n = 2, 6, 10).

IT **65605-33-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and deblocking of)

RN 65605-33-6 CAPLUS

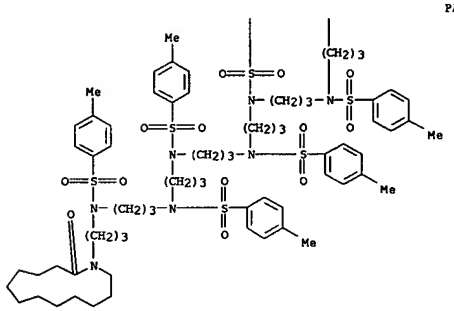
CN Benzenesulfonamide, 4-methyl-N-[4,8,12,16-tetrakis[(4-methylphenyl)sulfonyl]-19-(2-oxoazacyclotridec-1-yl)-4,8,12,16-tetraazanonadec-1-yl]-N-[4,8,12,16-tetrakis[(4-methylphenyl)sulfonyl]-21-phenyl-20-(phenylmethyl)-4,8,12,16,20-pentaazaheneicos-1-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

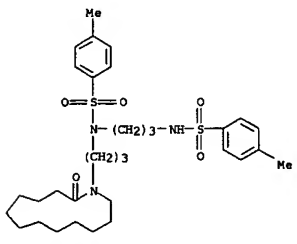
PAGE 2-A



IT **65545-59-7P 65605-32-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with phthalimidotricosyltriazapentadecane)

RN 65545-59-7 CAPLUS

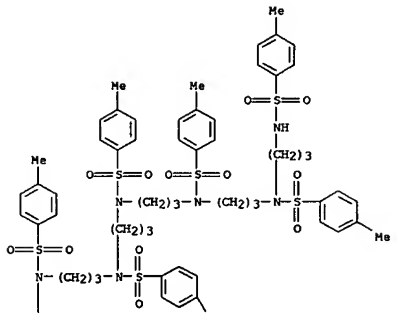
CN Benzenesulfonamide, 4-methyl-N-[3-[[(4-methylphenyl)sulfonyl]amino]propyl]-N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



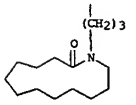
RN 65605-32-5 CAPLUS

CN Benzenesulfonamide, 4-methyl-N-[3-[[(4-methylphenyl)sulfonyl][3-[[[(4-methylphenyl)sulfonyl]amino]propyl]amino]propyl]-N-[3-[[(4-methylphenyl)sulfonyl][3-[[[(4-methylphenyl)sulfonyl][3-[[(4-methylphenyl)sulfonyl][3-[(2-oxoazacyclotridec-1-yl)amino]propyl]amino]propyl]amino]propyl]amino]propyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

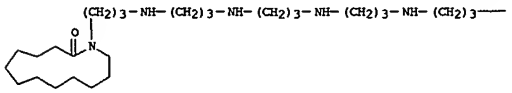


IT **65605-34-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and rearrangement of)

RN 65605-34-7 CAPLUS

CN Azacyclotridecan-2-one, 1-(39-amino-4,8,12,16,20,24,28,32,36-nonaazanonatriacont-1-yl)- (9CI) (CA INDEX NAME)

PAGE 1-A

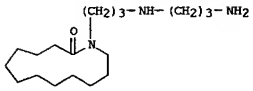


L4 ANSWER 22 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 1-B

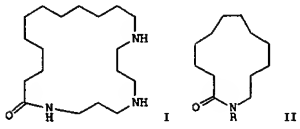
—NH—$(CH_2)_3$—NH—$(CH_2)_3$—NH—$(CH_2)_3$—NH—$(CH_2)_3$—NH—$(CH_2)_3$—NH_2

L4 ANSWER 23 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



L4 ANSWER 23 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1978:37595 CAPLUS
DOCUMENT NUMBER: 88:37595
TITLE: Transamidation reactions. 2. The "zip" reaction: a new method for ring enlargement; synthesis of 17- and 21-membered polyaminolactams
AUTHOR(S): Kramer, Urs; Guggisberg, Armin; Hesse, Manfred; Schmid, Hans
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, Switz.
SOURCE: Angewandte Chemie (1977), 89(12), 899-900
CODEN: ANCEAD; ISSN: 0044-8249
DOCUMENT TYPE: Journal
LANGUAGE: German
GI

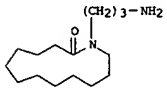


I II

AB Triazacycloheneicosanone I was prepd. by treating the azacyclotridecanone II (R = Na) with CH2:CHCN and hydrogenation of II (R = CH2CH2CN) to give 82% II [R = (CH2)3NH2]. Repetition of the sequence gave 78% II [R = (CH2)3NH(CH2)3NH2], which on treatment with KNH(CH2)3NH2 gave 90% I.

IT **64414-61-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with acrylonitrile)

RN 64414-61-5 CAPLUS
CN Azacyclotridecan-2-one, 1-(3-aminopropyl)- (9CI) (CA INDEX NAME)



IT **64414-60-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and rearrangement of, with aminopropylamide)

RN 64414-60-4 CAPLUS
CN Azacyclotridecan-2-one, 1-[3-[(3-aminopropyl)amino]propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 24 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1975:548304 CAPLUS
DOCUMENT NUMBER: 83:148304
TITLE: Polyamides with improved dyeability
INVENTOR(S): Ikeda, Masataka; Kusunose, Tetsuhiro; Shima, Tsukasa; Endo, Yumio; Kitamura, Kazuyuki
PATENT ASSIGNEE(S): Asahi Chemical Industry Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

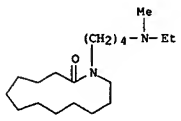
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 50043195	A2	19750418	JP 1973-92924	19730821

PRIORITY APPLN. INFO.: JP 1973-92924 19730821

AB Polyamide-forming substances were polycondensed with N-substituted lactams, esp. N-(N',N'-dimethylaminoethyl)caprolactam (I), N-(N'-methyl-N'-ethylaminopropyl)caprolactam [56525-26-9], and N-(N'-methyl-N'-ethylaminobutyl)laurolactam [**56525-27-0**]. Thus, hexamethylenediammonium adipate 120, I 0.57, and H2O 50 parts were heated at 230.degree. in N, then at 240.degree. and 17.5 kg/cm2, depressurized at 280.degree. during 1 hr to 0 kg/cm2 gage pressure, and polymd. further under N to give polyamide [56529-21-6] showing no color change during 5 hr standing at 280.degree. in N.

IT **56525-27-0**
RL: USES (Uses)
(polyamides modified by, with improved dyeability and heat stability)

RN 56525-27-0 CAPLUS
CN Azacyclotridecan-2-one, 1-[4-(ethylmethylamino)butyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1963:462243 CAPLUS
DOCUMENT NUMBER: 59:62243
ORIGINAL REFERENCE NO.: 59:11456d-h,11457a-b
TITLE: Guanidines
INVENTOR(S): Mull, Robert P.
PATENT ASSIGNEE(S): CIBA Ltd.
SOURCE: 5 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CH 365079		19621215	CH	
PRIORITY APPLN. INFO.:			US	19590610

GI For diagram(s), see printed CA Issue.
AB To a mixt. of 22.6 g. heptamethylenimine and 200 ml. C6H6 is added with stirring 13.6 g. chloroacetylguanide, the mixt. warmed 1 hr., cooled, filtered, the filtrate evapd. in vacuo, the crude heptamethyleniminoacetylguanide suspended in tetrahydrofuran (THF) and heated to reflux. to yield I (m = 3, n = 2).H2SO4, (II.H2SO4), m. 276-81.degree. (decompn.) (aq. EtOH). The same procedure is used to prep. the following sulfates of I [m, n, and m.p. (decompn.) given]: 1, 2, 203-7.degree.; 6, 2, 260 73.degree.; 4, 2, 272-5.degree.; 2, 2, 233-6.degree.; 3, 3, 248-52.degree.. To a soln. of 56.5 g. caprolactam and 28 g. acrylonitrile in 150 ml. dioxane is added with stirring a few drops of a strong base, such as PhCH2NMe3OH. The temp. is kept between 30-5.degree. for 30 min. and the reaction mixt. kept at room temp. for several days. The mixt. is acidified with HCl, evapd., and the residue distd. in vacuo to yield .beta.-(2-oxohexamethylenimino)propionitrile, b0.03 133-6.degree.. .beta.-(2-Oxohexamethylenimino)propionitrile (16.6 g.) is dissolved in abs. EtOH, 2 g. Raney Ni added, and the mixt. hydrogenated under pressure at 125.degree.. After the required amt. of H is taken up, the mixt. is cooled, the catalyst removed by filtration, and 13.9 g. S-methylisothiourea sulfate added. The mixt. is refluxed until no further MeSH is evolved, evapd. in vacuo, the residue taken into H2O, made alk. with aq. NaOH, extd. with Et2O, and the ext. dried. The resulting ether soln. of 3-(2-oxohexamethylenimino)propylguanidine is added to a mixt. of 5 g. LiAlH4 in 500 ml. Et2O and the reaction mixt. refluxed overnight. The excess LiAlH4 is decompd. by the addn. of H2O and aq. NaOH, filtered, the filtrate evapd., and the residue treated with dil. H2SO4 to yield 3-hexamethyleniminopropylguanidine. I and their salts lower blood pressure and can be used in the treatment of neurogenic or renal hypertension, especially when m = 3. Swiss 365,080 (Cl. 12p); 5 pp. To mixt. of 10.5 g. of HOCH2CH2NHC(:NH)NH2. HCl in 500 ml. PhMe is added 16.9 g. SOCl2. The mixt. is kept overnight, the solvent decanted, the excess SOCl2 and PhMe removed by evapn., and the residue extd. with EtOH-Et2O to give ClCH2CH2NHC(:NH)NH2.HCl (I.HCl). I.HCl yields I on the addn. of a stoichiometric amt. of NH3 in ether. I.HCl (15.8 g.) in EtOH is added to 22.6 g. heptamethylenimine (II) in 75 ml. EtOH, the mixt. heated several hrs. to boiling, cooled, filtered, and the filtrate evapd. in vacuo. The residue is dissolved in H2O, made alk. with dil. NaOH, and H2SO4 is added to yield III sulfate (n = 2, m = 4) (IV sulfate), m. 276-81.degree. (decompn.). In a similar manner III sulfate (n = 3, m = 4), m. 248-52.degree., is prepd. from II and Cl(CH2)3NHC(:NH)NH2.HCl.

L4 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

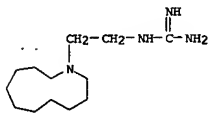
L4 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
Similarly are prepd, the following III sulfates [m, n, and m.p. (decompn.) given]: 2, 2, 205-7.degree.; 3, 2 (V), 233-6.degree.; 5, 2,272-5.degree.; 7, 2,26073.degree. (cf., CA 46, 7364e). A mixt. of 26.3 g. hexamethylenimine (Va), 33.2 g. ethylene bromohydrin, 200 ml. C6H6, and 15 g. anhyd. Na2CO3 is stirred overnight at reflux, filtered, evapd. in vacuo, and distd. to give 2-hexamethyleniminoethanol (VI), b13 98-101.degree.. To a mixt. of 5.72 g. VI in 50 ml. C6H6 is added dropwise 5.12 g. SOCl2 in 150 ml. C6H6, the mixt. heated to boiling and then stirred for 2 hrs. The mixt. is cooled, the ppt. removed by filtration, and crystd. from MeOH-Et2O to yield 2-hexamethyleniminoethyl chloride-HCl (VII.HCl), m. 212-16.degree.. When II replaces Va in this reaction, 2-heptamethyleniminoethyl chloride-HCl is obtained. A mixt. of 19.8 g. of VII.HCl, 21.6 g. guanidine sulfate, and H2O, made alk. with dil. NaOH, is heated on a water bath and several addns. of NaOH made to neutralize the acid formed during the reaction. The mixt. is cooled, acidified with H2SO4, and evapd. in vacuo to yield V, m. 233-6.degree.. The compds. lower blood pressure and are useful in the treatment of neurogenic or renal hypertension.
IT **96749-52-9**, Guanidine, [2-(azacycloundec-1-yl)ethyl]-, sulfate (prepn. of)
RN 96749-52-9 CAPLUS
CN Guanidine, [2-(azacycloundec-1-yl)ethyl]-, sulfate (6CI, 7CI) (CA INDEX NAME)

CM 1

CRN 7664-93-9
CMF H2 O4 S

CM 2

CRN 4355-63-9
CMF C13 H28 N4



L4 ANSWER 26 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1962:483191 CAPLUS
DOCUMENT NUMBER: 57:83191
ORIGINAL REFERENCE NO.: 57:16578a-d
TITLE: Guanidine compounds
PATENT ASSIGNEE(S): CIBA Ltd.
SOURCE: 5 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 883282		19611129	GB	
PRIORITY APPLN. INFO.:			US	19580610

AB Alkylene-amino-lower alkyl guanidines in which the alkylene amino ring contg. 4-10 C atoms in the ring and the acyl derivs. thereof were prepd. Thus, to a soln. of 73 g. chloroacetonitrile in 500 ml. C6H6 were added 51.5 g. anhyd. Na2CO3 and a soln. of 122.7 g. octahydroazonine in 250 ml. C6H6, the mixt. refluxed for 4 hrs. with stirring, cooled, filtered, concd. and the oily residue distd. in vacuo. To a suspension of 44.5 g. LiAlH4 in 2 l. Et2O, a soln. of 139.2 g. octahydro-1-azoninylacetonitrile in 300 ml. Et2O was added with cooling, and the mixt. refluxed for 3 hrs. and stirred overnight. In succession, 40 ml. H2O, 500 ml. 20% aq. NaOH, and 125 ml. H2O were added while cooling, and the mixt. filtered, concd. and distd. in vacuo; 5 g. resulting 2-(octahydro-1-azoninyl)ethylamine was dissolved in 7 ml. H2O and the soln. treated with 4.1 g. S-methylisothiourea sulfate. The mixt. was refluxed 1.5 hrs., H2O added to a total vol. of 55 ml., and the solid material which sepd. on further refluxing, was filtered off after cooling and recrystd. from H2O, to yield 5.4 g. 2-(octahydro-1-azoninyl)ethylguanidine sulfate, m. 272-5.degree. (decompn.). Similarly, 3-(octahydro-1-azocinyl)propylguanidine sulfate, m. 248-52.degree. (alc.-Et2O and alc.-hexane), 2-(hexahydro-1-azepinyl)ethylguanidine sulfate, m. 233-6.degree. (alc.-Et2O), 2-piperidinoethylguanidine sulfate, m. 203-7.degree. (decompn.) (alc.-Et2O), and 2-(decamethylenimino)ethylguanidine sulfate, m. 26-73.degree. (decompn.) (alc.), were prepd.
IT **96749-52-9**, Guanidine, [2-(azacycloundec-1-yl)ethyl]-, sulfate (prepn. of)
RN 96749-52-9 CAPLUS
CN Guanidine, [2-(azacycloundec-1-yl)ethyl]-, sulfate (6CI, 7CI) (CA INDEX NAME)

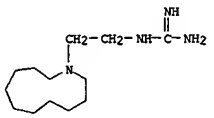
CM 1

CRN 7664-93-9
CMF H2 O4 S

CM 2

CRN 4355-63-9

L4 ANSWER 26 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
MF C13 H28 N4



L4 ANSWER 27 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1961:87110 CAPLUS
DOCUMENT NUMBER: 55:87110
ORIGINAL REFERENCE NO.: 55:16418b-i,16419a-c
TITLE: Guanidines with antihypertensive activity
AUTHOR(S): Mull, Robert P.; Egbert, Mary E.; Dapero, Mary R.
CORPORATE SOURCE: Ciba Pharm. Prods., Inc., Summit, NJ
SOURCE: Journal of Organic Chemistry (1960), 25, 1953-6
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. CA 53, 1538i. Guanethidine, [R(CH2)nNHC(:NH)NH2]2.H2SO4 (I) [R = octahydro-1-azocinyl (C7H14), n = 2] (II), was found to have protracted anti-hypertensive properties with the capacity to block sympathetic efferent transmission, presumably at the nerve terminals. The ring, side chain, and terminal groupings were altered and the relationship of these modifications to physiol. activity ascertained. The nitriles, R(CH2)nCN (III) were readily synthesized by condensation of an aliphatic or cyclic imine with a halo nitrile. The prepn. of the larger ring systems was previously described with exception of 1,4-hexahydrothiazepine (IV). Tetrahydro-1-thiopyran-4-one (15 g.) in 65 ml. cold concd. HCl stirred with slow addn. of 12.7 g. NaN3 and the mixt. stirred 4 hrs. at 20.degree., made slightly alk. with solid Na2CO3 and sufficient H2O to maintain soln., extd. with CHCl3 and the concd. ext. dild. with petr. ether yielded 62% hexahydro-5-oxo-1,4-thiazepine, m. 115-18.degree. (CCl4-C7H16). LiAlH4 (5.9 g.) in 800 ml. Et2O stirred with addn. of 12 g. solid lactam and the mixt. refluxed 24 hrs., carefully decompd. with 20 ml. H2O and the filtered soln. concd. yielded 88% IV, b. 192-3.degree., n27D 1.5342; HCl salt m. 210.degree.. Octahydroazocine (109.2 g.) in 280 ml. C6H6 stirred with 73 g. ClCH2CN and 51.5 g. anhyd. Na2CO3 in 500 ml C6H6, the mixt. refluxed 4 hrs., cooled, and the filtered soln. concd. in vacuo gave 87% III (R = C7H14N, n = 1) (V), b14 114-18.degree., n24D 1.4720. Similarly were prepd. previously non-reported nitriles III (R, n, % yield, b.p./mm., and nD/t.degree. given): C7H14N, 3, 71, 140-4.degree./15, 1.4751/28.degree.; C8H16N, 1, 120-5.degree./13, 1.4783/27.degree.; 1-azacycloundecyl (C10H20N), 1, 63, 149-53.degree./15, 1.4849/25.degree.; hexahydro-1,4-thiazepin-4-yl (C5H10NS), 1, 56, 148-50.degree./13, 1.5268/24. V (127.5 g.) in 300 ml. Et2O added slowly with stirring to 44.5 g. LiAlH4 in 2 l. Et2O and the mixt. refluxed 3 hrs., stirred at 20.degree. 16 hrs. and the cooled soln. decompd. by careful addn. of 40 ml. H2O, 50 ml. 20% NaOH, and 125 ml. H2O, filtered, and the Et2O layer evapd. gave 89% amine, R(CH2)nNH2 (VI, R = C7H14N, n = 2) (VII), b14 108-11.degree., n22D 1.4830. Similar LiAlH4 reduction of III gave the corresponding amines VI (R, n, % yield, b.p./mm., and nD/t.degree. given): C7H14N, 3, 70, 94-8.degree./0.4, 1.4858-25.degree.; C7H14N, 4, 74, 70-7.degree./0.35, 1.4818/28.degree.; C8H16N, 2, 76, 64-8.degree./0.7, 1.4859/26.degree.; C10H20N, 2, 70, 87-90.degree./0.3, 1.4880/28.degree.; C5H10NS, 2, 33, 120-2.degree./13, 1.5293/24.degree.. In general the guanidines were prepd. from the appropriate amine and a 2-methylthiopseudourea (VIII) salt. VIII.H2SO4 (86 g.) and 98 g. VII refluxed 8 hrs. in 300 ml. H2O with vigorous evolution of MeSH and the cooled solid recrystd. from EtOH-H2O yielded 74% II, m. 276-81.degree. (all crystns. from EtOH-H2O unless otherwise noted). Similarly were prepd. the listed I (R, n, % yield, and m.p. (decompn.) given): 1-pyrrolidinyl, 2, 80, 159-62.degree.; piperidino, 2, 53, 204-7.degree.; hexahydro-1-azepinyl, 2, 83, 208-15.degree.; C7H14N, 3, 82,

L4 ANSWER 27 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
248-52.degree.; C7H14N, 4, 66, 215-35.degree. (monohydrate, crystd. from EtOH); C8H16N, 2, 70, 272-5.degree.; C10H20N, 2, 70, 260-73.degree.; C5H10NS, 2, 63, 207-14.degree.; morpholino, 2, 41, 177-89.degree.; 10-phenothiazinyl, 3, 52, 127-30.degree.; 2-pyridyl, 2, 48, 147-50.degree.; 4-pyridyl, 2, 56, 256-7.degree.; Et2N, 2, 66, 210-15.degree. (alc.-Et2O); Bu2N, 2, 63, 120-3.degree. (H2O); Pr2N, 2, 73, 190-205.degree. (alc.-Et2O). PhCHBrCOMe (36.2 g.) in 100 ml. C6H6 added slowly with stirring to 38 g. C7H14NH in 125 ml. C6H6 and the mixt. refluxed 3 hrs., stirred 21 hrs. at 20.degree. and the filtered soln. concd. in vacuo yielded 30% 1-(octahydro-1-azocinyl)-1-phenyl-2-propanone, b0.4 115-28.degree., n28D 1.5312; oxime (IX), m. 85-8.degree. (alc.-H2O). IX (13.38 g.) in 100 ml. Et2O added with stirring to 4.35 g. LiAlH4 in 150 ml. Et2O under reflux and the mixt. refluxed 3 hrs., decompd. by addn. of 10 ml. H2O, 12 ml. 20% NaOH, and 30 ml. H2O, the filtered soln. concd. and the residual oil fractionated yielded 51% 1-methyl-2-(octahydro-1-azocinyl)-2-phenethylamine (X), b0.6 136-46.degree., n28D 1.5353. X (5 g.) and 2.83 g. VIII. H2SO4 refluxed in H2O and the solid recrystd. from alc.-Et2O yielded 61% cryst. [1-methyl-2-(octahydro-1-azocinyl)phenethyl]guanidine sulfate, m. 145-55.degree. (decompn.). VII (4 g.) in 10 ml. H2O warmed on a steam bath with 6.26 g. 2-methylthio-2-imidazoline HI salt until evolution of MeSH ceased, the oily product taken up in alc. and repptd. with Et2O yielded 67% [2-(octahydro-1-azocinyl)ethylamino]-2-imidazoline HI salt. (H2N)2CS (0.8 g.) in 26 ml. alc. stirred with addn. of 2 g. 2-(octahydro-1-azocinyl)ethylchloride HCl salt and the mixt. refluxed 6 hrs. yielded 56% [2-(octahydro-1-azocinyl)ethyl]-2-thiopseudourea-2HCl, m. 212-15.degree.. Guanidine compds. with 8-membered rings had max. physiol. activity. Of other ring systems only the pyridyl had noteworthy activity and the dialkylaminoalkyl guanidine were inactive. For optimal activity the Et side chain was essential. Replacement of the guanidino portion of the mol. by other functional groups gave inactive compds.

IT **96749-52-9**, Guanidine, (2-azacycloundec-1-ylethyl)-, sulfate
109098-16-0, Azacycloundecane, 1-(2-aminoethyl)-
(prepn. of)

RN 96749-52-9 CAPLUS
CN Guanidine, [2-(azacycloundec-1-yl)ethyl]-, sulfate (6CI, 7CI) (CA INDEX NAME)

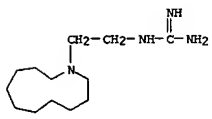
CM 1

CRN 7664-93-9
CMF H2 O4 S

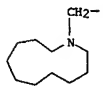
CM 2

CRN 4355-63-9
CMF C13 H28 N4

L4 ANSWER 27 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



RN 109098-16-0 CAPLUS
CN Azacycloundecane, 1-(2-aminoethyl)- (6CI) (CA INDEX NAME)

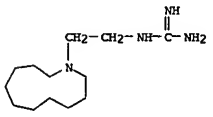


L4 ANSWER 28 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1960:91835 CAPLUS
DOCUMENT NUMBER: 54:91835
ORIGINAL REFERENCE NO.: 54:17436c-i,17437a-c
TITLE: Alkyleneimino lower alkylguanidines
INVENTOR(S): Mull, Robert P.
PATENT ASSIGNEE(S): Ciba Pharmaceutical Products, Inc.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2928829		19600315	US	
DE 1100637			DE	

AB N,N-Alkyleneimino lower alkyl guanidines, in which the alkyleneimino contained 4-10 C atoms as ring members, and their acid addn. salts as well as quaternary ammonium compds. were prepd. 2-(N,N-Heptamethyleneimino)ethylamine (Ia) (98 g.) in 300 ml. H2O heated 8 hrs. with 87 g. S-methylisothiourea sulfate gave 113.7 g. 2-(N,N-heptamethyleneimino)ethylguanidine sulfate (I), m. 276-81.degree. (decompn.). A concd. aq. soln. of I with a strong quaternary ammonium resin gave the free base. Addn. of alc. and Et2O satd. with HCl gave I.HCl. The starting material was prepd. as follows: 73 g. ClCH2CN in 500 ml. C6H6 treated with 51.5 g. anhyd. Na2CO3 and 109.2 g. N,N-heptamethyleneimine in 250 ml. C6H6, the mixt. refluxed 4 hrs., cooled, and the residue distd. gave 127.5 g. (N,N-heptamethyleneimino)acetonitrile (II), b14 114-18.degree.. LiAlH4 (44.5 g.) and 2 l. Et2O treated with 127.5 g. II in 300 ml. Et2O, the soln. refluxed 3 hrs., stirred overnight, and decompd. gave 115.7 g. Ia, b14 108-11.degree.. 3-(N,N-Heptamethyleneimino)propylamine (III) (5 g.) in 10 ml. H2O heated 4 hrs. with 4.1 g. S-methyl-isothiourea sulfate gave 6.3 g. 3-(N,N-heptamethyleneimino)propylguanidine sulfate, m. 248-52.degree. (decompn.). N,N-Heptamethyleneimine (14.3 g.) added to 27.6 g. acrylonitrile, 2 ml. 38% aq. trimethylbenzylammonium hydroxide added, the mixt. stirred overnight at room temp., and distd. gave 3-(N,N-heptamethyleneimino)propionitrile (IV), b0.9 94-7.degree.. Redn. of IV with LiAlH4 gave III. N,N-Octamethyleneimine treated with ClCH2CN and the resulting nitrile reduced with LiAlH4 gave 2-(N,N-octamethyleneimino)ethylamine (V). V (5 g.) in 7 ml. H2O refluxed 1.5 hrs. with 4.1 g. S-methyl-isothiourea sulfate gave 5.4 g. 2-(N,N-octamethyleneimino)ethylguanidine sulfate, m. 272-5.degree. (decompn.). 2-(N,N-Hexamethyleneimino)ethylamine (5 g.) and 4.9 g. S-methylisothiourea sulfate in 10 ml. H2O refluxed 7 hrs. gave 6.8 g. 2-(N,N-hexamethyleneimino)ethylguanidine sulfate (VI), m. 233-6.degree. (decompn.). VI in H2O filtered through a column contg. a strong anion exchange resin gave a product which treated with HCl gave 2-(N,N-hexamethyleneimino)ethylguanidine-HCl; the methiodide was similarly obtained. 2-(N,N-Pentamethyleneimino)ethylamine (5 g.) in 7 ml. H2O warmed with 5.45 g. S-methylisothiourea sulfate gave 4.5 g. 2-(N,N-pentamethyleneimino)ethylguanidine sulfate, m. 203-7.degree. (decompn.). 2-(N,N-Tetramethyleneimino)ethylguanidine sulfate was similarly obtained. 2-(N,N-Decamethyleneimino)ethylamine (2.5 g.) in 5 ml. H2O heated 4 hrs. with 1.76 g. S-methylisothiourea sulfate gave 2.3 g. 2-(N,N-decamethyleneimino)ethylguanidine sulfate, m. 260-73.degree.

L4 ANSWER 28 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



L4 ANSWER 28 OF 28 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
(decompn.). N,N-Heptamethyleneimine (13.79 g.) in 50 ml. C6H6 treated with 15.3 g. 2-bromoethanol and 6.5 g. Na2CO3, the mixt. refluxed 17 hrs., cooled, and distd. gave 14.78 g. 2-(N,N-heptamethyleneimino)ethanol (VII), b14 110-15.degree.. VII (6.28 g.) in 50 ml. C6H6 refluxed 2 hrs. with 5.2 g. SOCl2 in 150 ml. C6H6 and the product recrystd. gave 4 g. 2-(N,N-heptamethyleneimino)ethyl chloride-HCl (VIII), m. 204-5.degree. (MeOH). VIII (10.22 g.) refluxed 3 hrs. with 17.5 g. 33% alc. and MeNH2 in the presence of 5.5 g. K2CO3 gave 3.1 g. N-[2-(N,N-heptamethyleneimino)ethyl]-N-methylamine (IX), b13 99-101.degree., n27D 1.4719. IX (3.1 g.) and 2.54 g. S-methylisothiourea sulfate in 5 ml. H2O refluxed 4 hrs. gave 2.2 g. 3-[2-(N,N-heptamethyleneimino)ethyl]-3-methylguanidine sulfate, m. 284-6.degree. (decompn.). 1-Guanyl-3,5-dimethylpyrazole nitrate (2.01 g.) and 15.6 g. Ia refluxed 2.5 hrs. and the product treated with a strong anion exchange resin gave I. Ia.2HCl (11.45 g.) and 3.15 g. cyanamide in 100 ml. alc. refluxed 6 hrs. gave I by the aid of a strong anion exchange resin. Ia (5 g.) in 10 ml. H2O heated with 4.5 g. 1-methyl-S-methylisothiourea sulfate gave 3-[2-(N,N-heptamethyleneimino)ethyl]-1-methylguanidine sulfate. Benzoyl cyanamide (1.46 g.) and 1.56 g. Ia treated with concd. HCl, the mixt. heated 10-15 min., and the product sepd. gave 1-benzoyl-3-[2-(N,N-heptamethyleneimino)ethyl]guanidine HCl, .nu. 1678 cm.-1 I.HCl (2.35 g.) and 1 g. propionyl chloride heated several hrs. at 105.degree. in a sealed tube gave 3-[2(N,N-heptamethyleneimino)ethyl]-1-propionylguanidine-HCl. I.HCl (2.35 g.) similarly with 0.8 g. AcCl gave 1-acetyl-3-[2-(N,N-heptamethyleneimino)ethyl]guanidine HCl. 4-Methyl-N,N-hexamethyleneimine with acrylonitrile in the presence of benzyltrimethylammonium hydroxide gave 3-(4-methyl-N,N-hexamethyleneimino)propionitrile (X), b15 126-30.degree.. Redn. of X with LiAlH4 gave 3-(4-methyl-N,N-hexamethyleneimino)propylamine (XI). XI in H2O treated with S-methylisothiourea gave 3-(4-methyl-N,N-hexamethyleneimino)propylguanidine sulfate.

IT **96749-52-9**, Guanidine, (2-azacycloundec-1-ylethyl)-, sulfate (prepn. of)

RN 96749-52-9 CAPLUS

CN Guanidine, [2-(azacycloundec-1-yl)ethyl]-, sulfate (6CI, 7CI) (CA INDEX NAME)

CM 1

CRN 7664-93-9
CMF H2 O4 S

CM 2

CRN 4355-63-9
CMF C13 H28 N4

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	142.18	290.54

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-19.53	-19.53

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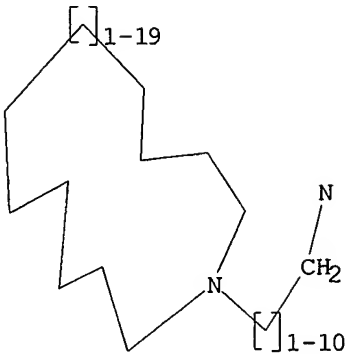

Structure attributes must be viewed using STN Express query preparation.

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                        BATCH   **COMPLETE**
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PROJECTED ANSWERS:             143 TO      194

L3           143 SEA SSS FUL L1

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COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                                148.15     148.36

FILE 'CAPLUS' ENTERED AT 16:57:53 ON 06 AUG 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 6 Aug 2003 VOL 139 ISS 6
FILE LAST UPDATED: 5 Aug 2003 (20030805/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 23 L3

=> s l4 and angiogenesis?
L5 3 L4 AND ANGIOGENESIS?

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L5 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:574910 CAPLUS
DOCUMENT NUMBER: 137:119652
TITLE: Antiangiogenic compounds and an assay for inhibitors of cell invasion
INVENTOR(S): Roskelley, Calvin; Andersen, Raymond; Williams, David; Roberge, Michel; Dedhar, Shoukat; Karsan, Aly; Minchinton, Andrew
PATENT ASSIGNEE(S): The University of British Columbia, Can.
SOURCE: PCT Int. Appl., 56 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002058679	A2	20020801	WO 2002-CA97	20020125
WO 2002058679	A3	20030515		

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US 2003004149	A1	20030102	US 2002-57846	20020125
PRIORITY APPLN. INFO.:			CA 2001-2332138 A	20010125
			US 2001-330670P P	20011026

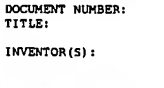
OTHER SOURCE(S): MARPAT 137:119652

AB This invention provides the use of macrocyclic amines for inhibition of cellular invasion or **angiogenesis**. Compds. and pharmaceutical compns. of this invention are useful in the treatment of conditions characterized by cellular invasion or **angiogenesis**, including cancer. Compds. that may be used in this invention include the motuporamines, which are isolated from methanol exts. of Xestospongia exigua.

IT **398144-70-2**, Motuporamine G **398144-76-8**, Motuporamine H **398144-77-9**, Motuporamine I
RL: NPO (Natural product occurrence); BIOL (Biological study); OCCU (Occurrence)
(antiangiogenic macrocyclic amines and assays for inhibitors of cell invasion)

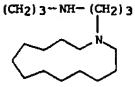
RN 398144-70-2 CAPLUS
CN 1,3-Propanediamine, N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

L5 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



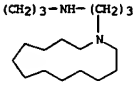
D1-Me

RN 398144-76-8 CAPLUS
CN 1,3-Propanediamine, N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



D1-Me

RN 398144-77-9 CAPLUS
CN 1,3-Propanediamine, N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

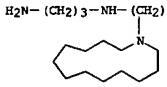


D1-Me

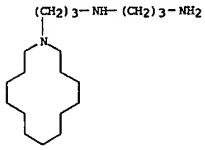
IT **211566-77-7**, Motuporamine A **211566-78-8**, Motuporamine B **211569-34-5**, Motuporamine C
RL: NPO (Natural product occurrence); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES (Uses)
(antiangiogenic macrocyclic amines and assays for inhibitors of cell invasion)

RN 211566-77-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)

L5 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

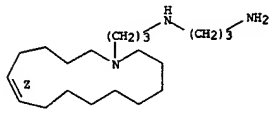


RN 211566-78-8 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)



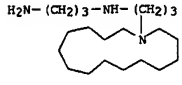
RN 211569-34-5 CAPLUS
CN 1,3-Propanediamine, N-[3-[(6Z)-azacyclopentadec-6-en-1-yl]propyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IT **211569-33-4**, Dihydromotuporamine C **251349-16-3**, Diacetyl motuporamine C **385437-34-3** **397262-93-0**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antiangiogenic macrocyclic amines and assays for inhibitors of cell invasion)

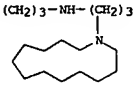
RN 211569-33-4 CAPLUS
CN 1,3-Propanediamine, N-[3-(azacyclopentadec-1-yl)propyl]- (9CI) (CA INDEX NAME)



L5 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

D1-Me

RN 398144-76-8 CAPLUS
CN 1,3-Propanediamine, N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



D1-Me

RN 398144-77-9 CAPLUS
CN 1,3-Propanediamine, N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

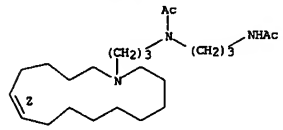
D1-Me

IT **211566-77-7**, Motuporamine A **211566-78-8**, Motuporamine B **211569-34-5**, Motuporamine C
RL: NPO (Natural product occurrence); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES (Uses)
(antiangiogenic macrocyclic amines and assays for inhibitors of cell invasion)

RN 211566-77-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)

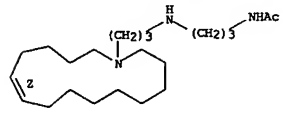
L5 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
RN 251349-16-3 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



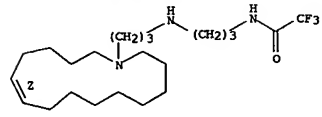
RN 385437-34-3 CAPLUS
CN Acetamide, N-[3-[[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]amino]propyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 397262-93-0 CAPLUS
CN Acetamide, N-[3-[[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]amino]propyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:893633 CAPLUS
DOCUMENT NUMBER: 136:164301
TITLE: Motuporamines, anti-invasion and anti-angiogenic alkaloids from the marine sponge Xestospongia exigua (Kirkpatrick): Isolation, structure elucidation, analogue synthesis, and conformational analysis
AUTHOR(S): Williams, David E.; Craig, Kyle S.; Patrick, Brian; McHardy, Lianne M.; van Soest, Rob; Roberge, Michel; Andersen, Raymond J.
CORPORATE SOURCE: Departments of Chemistry Oceanography (EOS) Biochemistry and Molecular Biology, University of British Columbia, Vancouver, BC, Can.
SOURCE: Journal of Organic Chemistry (2002), 67(1), 245-258 CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

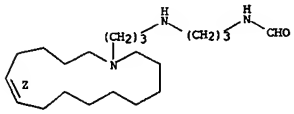
AB Exts. of the sponge Xestospongia exigua collected in Papua New Guinea were pos. in a new assay for anti-invasion activity. Bioassay-guided fractionation led to the identification of the three known motuporamines A, B, and C along with the new motuporamines D (e.g. I), E, and F and a mixt. of G, H, and I. Motuporamines A, B, and C and the mixt. of G, H, and I were responsible for the anti-invasion activity of the crude ext. Motuporamine C has also been found to be anti-angiogenic. A series of analogs of the motuporamines have been synthesized and evaluated for anti-invasive activity. These SAR results revealed that a satd. 15-membered cyclic amine fused to the natural motuporamine diamine side chain (II) represented the optimal structure for anti-invasive activity in this family. Single-crystal X-ray diffraction anal. of one of the analogs (III) showed that in the solid state its 16-membered macrocyclic amine fragment adopted the [4444] quadrangular conformation predicted by calcns. to be the lowest energy conformation for the corresponding cycloalkane, cyclohexadecane. These data along with literature X-ray data and conformational anal. for derivs. of azacyclotridecane have been used as precedents for predicting the lowest energy ring conformations of other motuporamines. The SAR data from the natural and synthetic motuporamines have been combined with the conformational analyses to provide an outline of the functionality and shape required for activity in this family of alkaloids and to design a new analog (IV) that showed good anti-invasion activity.

IT **211566-77-7**, Motuporamine A **211566-78-8**, Motuporamine B **211569-34-5**, Motuporamine C
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); BIOL (Biological study)
(anti-invasion and anti-angiogenic alkaloids from marine sponge Xestospongia exigua)

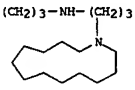
RN 211566-77-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)

L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

Double bond geometry as shown.

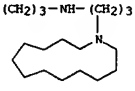


RN 398144-70-2 CAPLUS
CN 1,3-Propanediamine, N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



D1-Me

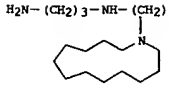
RN 398144-76-8 CAPLUS
CN 1,3-Propanediamine, N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



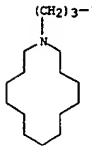
D1-Me

RN 398144-77-9 CAPLUS
CN 1,3-Propanediamine, N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
NAME)

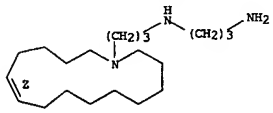


RN 211566-78-8 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)



RN 211569-34-5 CAPLUS
CN 1,3-Propanediamine, N-[3-[(6Z)-azacyclopentadec-6-en-1-yl]propyl]- (9CI) (CA INDEX NAME)

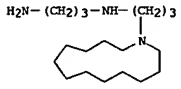
Double bond geometry as shown.



IT **398144-69-9P**, Motuporamine F **398144-70-2P**, Motuporamine G **398144-76-8P**, Motuporamine H **398144-77-9P**, Motuporamine I
RL: NPO (Natural product occurrence); PAC (Pharmacological activity); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(anti-invasion and anti-angiogenic alkaloids from marine sponge Xestospongia exigua)

RN 398144-69-9 CAPLUS
CN Formamide, N-[3-[[3-(6Z)-azacyclotridec-6-en-1-ylpropyl]amino]propyl]- (9CI) (CA INDEX NAME)

L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

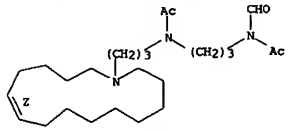


D1-Me

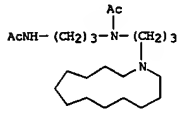
IT **397262-94-1P**, Diacetylmotuporamine F **398144-71-3P**, DiacetylMotuporamine G **398144-75-7P**, Diacetylmotuporamine H **398144-78-0P**, Diacetylmotuporamine I
RL: PRP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)
(anti-invasion and anti-angiogenic alkaloids from marine sponge Xestospongia exigua)

RN 397262-94-1 CAPLUS
CN Acetamide, N-[3-[acetyl[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]amino]propyl]-N-formyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



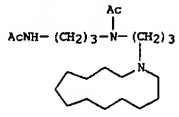
RN 398144-71-3 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



D1-Me

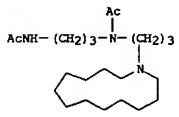
RN 398144-75-7 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



D1-Me

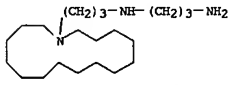
RN 398144-78-0 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



D1-Me

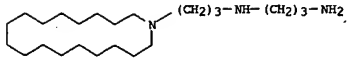
IT **397263-04-6P 397263-05-7P 397263-06-8P 397263-07-9P 397263-15-9P**, Azacyclotridecane-1-propanamine **397263-63-7P 397263-68-2P 397263-70-6P 397263-72-8P 397263-74-0P 397263-76-2P 397263-77-3P 397263-79-5P 397263-80-8P**
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(anti-invasive and antitumor activities of motuporamines and their analogs)

RN 397263-04-6 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclohexadec-1-ylpropyl)- (9CI) (CA INDEX NAME)



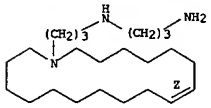
RN 397263-05-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclooctadec-1-ylpropyl)- (9CI) (CA INDEX

L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
NAME)



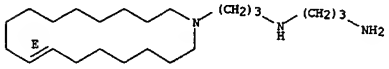
RN 397263-06-8 CAPLUS
CN 1,3-Propanediamine, N-[3-(8Z)-azacyclooctadec-8-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

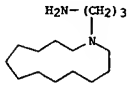


RN 397263-07-9 CAPLUS
CN 1,3-Propanediamine, N-[3-(8E)-azacyclooctadec-8-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

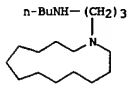


RN 397263-15-9 CAPLUS
CN Azacyclotridecane-1-propanamine (9CI) (CA INDEX NAME)

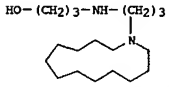


RN 397263-63-7 CAPLUS
CN Azacyclotridecane-1-propanamine, N-butyl- (9CI) (CA INDEX NAME)

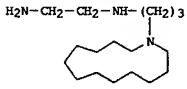
L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



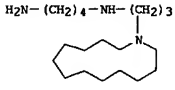
RN 397263-68-2 CAPLUS
CN 1-Propanol, 3-[(3-azacyclotridec-1-ylpropyl)amino]- (9CI) (CA INDEX NAME)



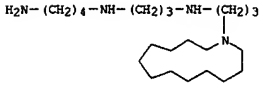
RN 397263-70-6 CAPLUS
CN 1,2-Ethanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)



RN 397263-72-8 CAPLUS
CN 1,4-Butanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)

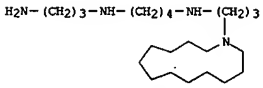


RN 397263-74-0 CAPLUS
CN 1,4-Butanediamine, N-[3-[(3-azacyclotridec-1-ylpropyl)amino]propyl]- (9CI) (CA INDEX NAME)

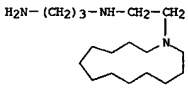


RN 397263-76-2 CAPLUS

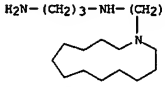
L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
CN 1,4-Butanediamine, N-(3-aminopropyl)-N'-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)



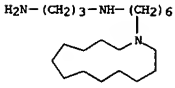
RN 397263-77-3 CAPLUS
CN 1,3-Propanediamine, N-(2-azacyclotridec-1-ylethyl)- (9CI) (CA INDEX NAME)



RN 397263-79-5 CAPLUS
CN 1,3-Propanediamine, N-(4-azacyclotridec-1-ylbutyl)- (9CI) (CA INDEX NAME)



RN 397263-80-8 CAPLUS
CN 1,3-Propanediamine, N-(6-azacyclotridec-1-ylhexyl)- (9CI) (CA INDEX NAME)

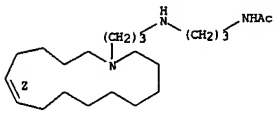


IT **385437-34-3 397262-93-0**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(artifact from marine sponge Xestospongia exigua)

RN 385437-34-3 CAPLUS
CN Acetamide, N-[3-[[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]amino]propyl]- (9CI) (CA INDEX NAME)

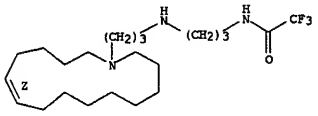
Double bond geometry as shown.

L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

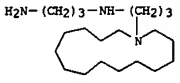


RN 397262-93-0 CAPLUS
CN Acetamide, N-[3-[[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]amino]propyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

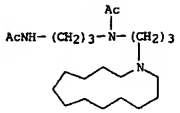


IT **211569-33-4P**, Dihydromotuporamine C
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and anti-invasive activity of)
RN 211569-33-4 CAPLUS
CN 1,3-Propanediamine, N-[3-(azacyclopentadec-1-yl)propyl]- (9CI) (CA INDEX NAME)

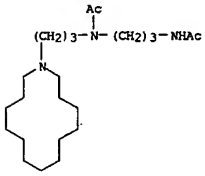


IT **211388-13-5P**, Diacetylmotuporamine A **211388-14-6P**, Diacetylmotuporamine B **251349-16-3P**, Diacetylmotuporamine C
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 211388-13-5 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)

L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

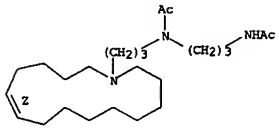


RN 211388-14-6 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)



RN 251349-16-3 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



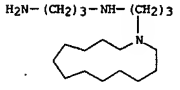
REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:712129 CAPLUS
DOCUMENT NUMBER: 136:63714
TITLE: Inhibition of tumor cell invasion and **angiogenesis** by motuporamines
AUTHOR(S): Roskelley, Calvin D.; Williams, David E.; McHardy, Lianne M.; Leong, Kevin G.; Troussard, Armelle; Karsan, Aly; Andersen, Raymond J.; Dedhar, Shoukat; Roberge, Michel
CORPORATE SOURCE: Departments of Anotomy, University of British Columbia, Vancouver, BC, V6T 1Z3, Can.
SOURCE: Cancer Research (2001), 61(18), 6788-6794
CODEN: CNREA8; ISSN: 0008-5472
PUBLISHER: American Association for Cancer Research
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Tissue invasion is an important determinant of **angiogenesis** and metastasis and constitutes an attractive target for cancer therapy. We have developed an assay to identify agents that inhibit invasion by mechanisms other than inhibition of cell attachment or cytotoxicity. A screen of marine sponge exts. identified motuporamines as micromolar inhibitors of invasion of basement membrane gels by MDA-231 breast carcinoma, PC-3 prostate carcinoma, and U-87 and U-251 glioma cells. Motuporamine C inhibits cell migration in monolayer cultures and impairs actin-mediated membrane ruffling at the leading edge of lamellae. Motuporamine C also reduces .beta.1-integrin activation, raising the possibility that it interferes with "inside-out" signaling to integrins. In addn., motuporamine C inhibits **angiogenesis** in an in vitro sprouting assay with human endothelial cells and an in vivo chick chorioallantoic membrane assay. The motuporamines show little or no toxicity or inhibition of cell proliferation, and they are structurally simple and easy to synthesize, making them attractive drug candidates.

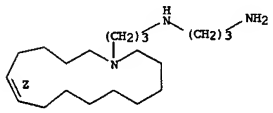
IT **211566-77-7**, Motuporamine A **211569-34-5**, Motuporamine C **251349-16-3 385437-34-3**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(inhibition of tumor cell invasion and **angiogenesis** by motuporamines)
RN 211566-77-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)



RN 211569-34-5 CAPLUS
CN 1,3-Propanediamine, N-[3-[(6Z)-azacyclopentadec-6-en-1-yl]propyl]- (9CI) (CA INDEX NAME)

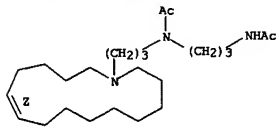
Double bond geometry as shown.

L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



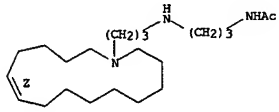
RN 251349-16-3 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 385437-34-3 CAPLUS
CN Acetamide, N-[3-[[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]amino]propyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d l4 ibib abs hitstr tot

L4 ANSWER 1 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:574910 CAPLUS
DOCUMENT NUMBER: 137:119652
TITLE: Antiangiogenic compounds and an assay for inhibitors of cell invasion
INVENTOR(S): Roskelley, Calvin; Andersen, Raymond; Williams, David; Roberge, Michel; Dedhar, Shoukat; Karsan, Aly; Minchinton, Andrew
PATENT ASSIGNEE(S): The University of British Columbia, Can.
SOURCE: PCT Int. Appl., 56 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002058679	A2	20020801	WO 2002-CA97	20020125
WO 2002058679	A3	20030515		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003004149	A1	20030102	US 2002-57846	20020125

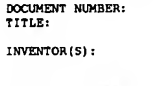
PRIORITY APPLN. INFO.: CA 2001-2332138 A 20010125
US 2001-330670P P 20011026
OTHER SOURCE(S): MARPAT 137:119652

AB This invention provides the use of macrocyclic amines for inhibition of cellular invasion or angiogenesis. Compds. and pharmaceutical compns. of this invention are useful in the treatment of conditions characterized by cellular invasion or angiogenesis, including cancer. Compds. that may be used in this invention include the motuporamines, which are isolated from methanol exts. of Xestospongia exigua.

IT **398144-70-2**, Motuporamine G **398144-76-8**, Motuporamine H
398144-77-9, Motuporamine I
RL: NPO (Natural product occurrence); BIOL (Biological study); OCCU (Occurrence)
(antiangiogenic macrocyclic amines and assays for inhibitors of cell invasion)

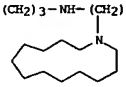
RN 398144-70-2 CAPLUS
CN 1,3-Propanediamine, N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



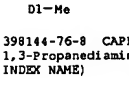
D1-Me

RN 398144-76-8 CAPLUS
CN 1,3-Propanediamine, N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



D1-Me

RN 398144-77-9 CAPLUS
CN 1,3-Propanediamine, N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

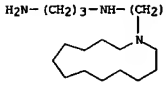


D1-Me

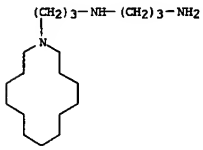
IT **211566-77-7**, Motuporamine A **211566-78-8**, Motuporamine B
211569-34-5, Motuporamine C
RL: NPO (Natural product occurrence); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES (Uses)
(antiangiogenic macrocyclic amines and assays for inhibitors of cell invasion)

RN 211566-77-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

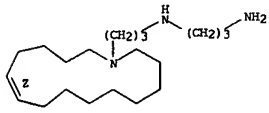


RN 211566-78-8 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)



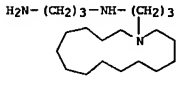
RN 211569-34-5 CAPLUS
CN 1,3-Propanediamine, N-[3-[(6Z)-azacyclopentadec-6-en-1-yl]propyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IT **211569-33-4**, Dihydromotuporamine C **251349-16-3**, Diacetyl motuporamine C **385437-34-3** **397262-93-0**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antiangiogenic macrocyclic amines and assays for inhibitors of cell invasion)

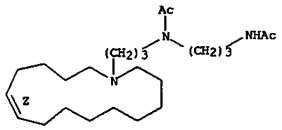
RN 211569-33-4 CAPLUS
CN 1,3-Propanediamine, N-[3-(azacyclopentadec-1-yl)propyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 1 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

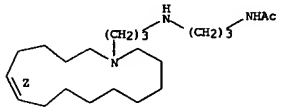
RN 251349-16-3 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



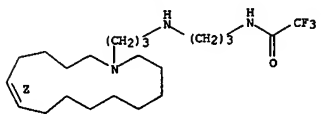
RN 385437-34-3 CAPLUS
CN Acetamide, N-[3-[[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]amino]propyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 397262-93-0 CAPLUS
CN Acetamide, N-[3-[[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]amino]propyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L4 ANSWER 2 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:893633 CAPLUS
DOCUMENT NUMBER: 136:164301
TITLE: Motuporamines, anti-invasion and anti-angiogenic alkaloids from the marine sponge Xestospongia exigua (Kirkpatrick): Isolation, structure elucidation, analogue synthesis, and conformational analysis
AUTHOR(S): Williams, David E.; Craig, Kyle S.; Patrick, Brian; McHardy, Lianne M.; van Soest, Rob; Roberge, Michel; Andersen, Raymond J.
CORPORATE SOURCE: Departments of Chemistry Oceanography (EOS) Biochemistry and Molecular Biology, University of British Columbia, Vancouver, BC, Can.
SOURCE: Journal of Organic Chemistry (2002), 67(1), 245-258 CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

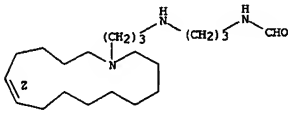
AB Exts. of the sponge Xestospongia exigua collected in Papua New Guinea were pos. in a new assay for anti-invasion activity. Bioassay-guided fractionation led to the identification of the three known motuporamines A, B, and C along with the new motuporamines D (e.g. I), E, and F and a mixt. of G, H, and I. Motuporamines A, B, and C and the mixt. of G, H, and I were responsible for the anti-invasion activity of the crude ext. Motuporamine C has also been found to be anti-angiogenic. A series of analogs of the motuporamines have been synthesized and evaluated for anti-invasive activity. These SAR results revealed that a satd. 15-membered cyclic amine fused to the natural motuporamine diamine side chain (II) represented the optimal structure for anti-invasive activity in this family. Single-crystal X-ray diffraction anal. of one of the analogs (III) showed that in the solid state its 16-membered macrocyclic amine fragment adopted the [4444] quadrangular conformation predicted by calcns. to be the lowest energy conformation for the corresponding cycloalkane, cyclohexadecane. These data along with literature X-ray data and conformational anal. for derivs. of azacyclotridecane have been used as precedents for predicting the lowest energy ring conformations of other motuporamines. The SAR data from the natural and synthetic motuporamines have been combined with the conformational analyses to provide an outline of the functionality and shape required for activity in this family of alkaloids and to design a new analog (IV) that showed good anti-invasion activity.

IT **211566-77-7**, Motuporamine A **211566-78-8**, Motuporamine B **211569-34-5**, Motuporamine C
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); BIOL (Biological study)
(anti-invasion and anti-angiogenic alkaloids from marine sponge Xestospongia exigua)

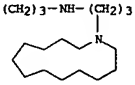
RN 211566-77-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX

L4 ANSWER 2 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

Double bond geometry as shown.

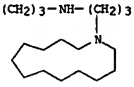


RN 398144-70-2 CAPLUS
CN 1,3-Propanediamine, N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



D1-Me

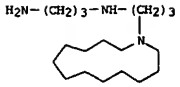
RN 398144-76-8 CAPLUS
CN 1,3-Propanediamine, N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



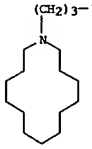
D1-Me

RN 398144-77-9 CAPLUS
CN 1,3-Propanediamine, N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
NAME)

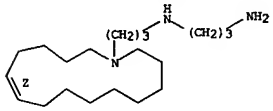


RN 211566-78-8 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)



RN 211569-34-5 CAPLUS
CN 1,3-Propanediamine, N-[3-[(6Z)-azacyclopentadec-6-en-1-yl]propyl]- (9CI) (CA INDEX NAME)

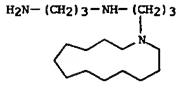
Double bond geometry as shown.



IT **398144-69-9P**, Motuporamine F **398144-70-2P**, Motuporamine G **398144-76-8P**, Motuporamine H **398144-77-9P**, Motuporamine I
RL: NPO (Natural product occurrence); PAC (Pharmacological activity); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(anti-invasion and anti-angiogenic alkaloids from marine sponge Xestospongia exigua)

RN 398144-69-9 CAPLUS
CN Formamide, N-[3-[[3-(6Z)-azacyclotridec-6-en-1-ylpropyl]amino]propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

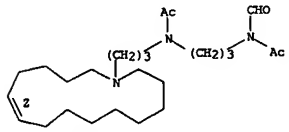


D1-Me

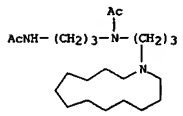
IT **397262-94-1P**, Diacetylmotuporamine F **398144-71-3P**, DiacetylMotuporamine G **398144-75-7P**, Diacetylmotuporamine H **398144-78-0P**, Diacetylmotuporamine I
RL: PRP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)
(anti-invasion and anti-angiogenic alkaloids from marine sponge Xestospongia exigua)

RN 397262-94-1 CAPLUS
CN Acetamide, N-[3-[acetyl[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]amino]propyl]-N-formyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



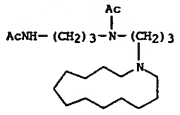
RN 398144-71-3 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



D1-Me

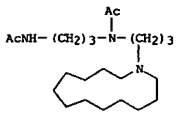
RN 398144-75-7 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



D1-Me

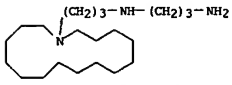
RN 398144-78-0 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(methylazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



D1-Me

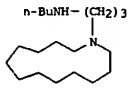
IT 397263-04-6P 397263-05-7P 397263-06-8P
397263-07-9P 397263-15-9P, Azacyclotridecane-1-propanamine 397263-63-7P 397263-68-2P
397263-70-6P 397263-72-8P 397263-74-0P
397263-76-2P 397263-77-3P 397263-79-5P
397263-80-8P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(anti-invasive and antitumor activities of motuporamines and their analogs)

RN 397263-04-6 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclohexadec-1-ylpropyl)- (9CI) (CA INDEX NAME)

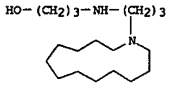


RN 397263-05-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclooctadec-1-ylpropyl)- (9CI) (CA INDEX

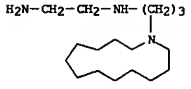
L4 ANSWER 2 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



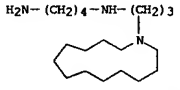
RN 397263-68-2 CAPLUS
CN 1-Propanol, 3-[(3-azacyclotridec-1-ylpropyl)amino]- (9CI) (CA INDEX NAME)



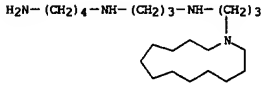
RN 397263-70-6 CAPLUS
CN 1,2-Ethanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)



RN 397263-72-8 CAPLUS
CN 1,4-Butanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)

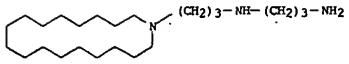


RN 397263-74-0 CAPLUS
CN 1,4-Butanediamine, N-[3-[(3-azacyclotridec-1-ylpropyl)amino]propyl]- (9CI) (CA INDEX NAME)



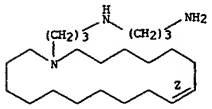
RN 397263-76-2 CAPLUS

L4 ANSWER 2 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
NAME)



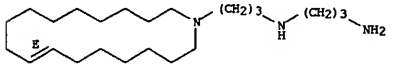
RN 397263-06-8 CAPLUS
CN 1,3-Propanediamine, N-[3-(8Z)-azacyclooctadec-8-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

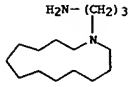


RN 397263-07-9 CAPLUS
CN 1,3-Propanediamine, N-[3-(8E)-azacyclooctadec-8-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

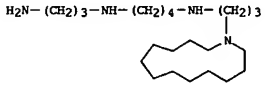


RN 397263-15-9 CAPLUS
CN Azacyclotridecane-1-propanamine (9CI) (CA INDEX NAME)

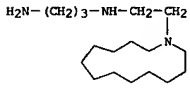


RN 397263-63-7 CAPLUS
CN Azacyclotridecane-1-propanamine, N-butyl- (9CI) (CA INDEX NAME)

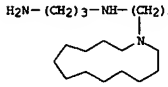
L4 ANSWER 2 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
CN 1,4-Butanediamine, N-(3-aminopropyl)-N'-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)



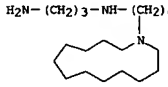
RN 397263-77-3 CAPLUS
CN 1,3-Propanediamine, N-(2-azacyclotridec-1-ylethyl)- (9CI) (CA INDEX NAME)



RN 397263-79-5 CAPLUS
CN 1,3-Propanediamine, N-(4-azacyclotridec-1-ylbutyl)- (9CI) (CA INDEX NAME)



RN 397263-80-8 CAPLUS
CN 1,3-Propanediamine, N-(6-azacyclotridec-1-ylhexyl)- (9CI) (CA INDEX NAME)

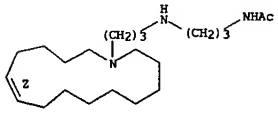


IT 385437-34-3 397262-93-0
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(artifact from marine sponge Xestospongia exigua)

RN 385437-34-3 CAPLUS
CN Acetamide, N-[3-[[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]amino]propyl]- (9CI) (CA INDEX NAME)

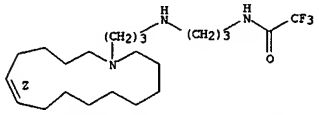
Double bond geometry as shown.

L4 ANSWER 2 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

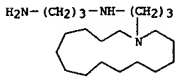


RN 397262-93-0 CAPLUS
CN Acetamide, N-[3-[[3-[(6Z)-azacyclopentadec-6-en-1-ylpropyl]amino]propyl]-2,2,2-trifluoro- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

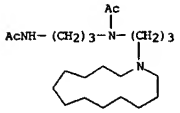


IT **211569-33-4P**, Dihydromotuporamine C
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and anti-invasive activity of)
RN 211569-33-4 CAPLUS
CN 1,3-Propanediamine, N-[3-(azacyclopentadec-1-yl)propyl]- (9CI) (CA INDEX NAME)

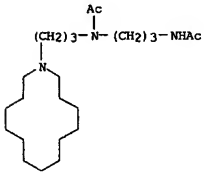


IT **211388-13-5P**, Diacetylmotuporamine A **211388-14-6P**, Diacetylmotuporamine B **251349-16-3P**, Diacetylmotuporamine C
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 211388-13-5 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

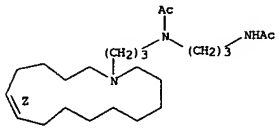


RN 211388-14-6 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)



RN 251349-16-3 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

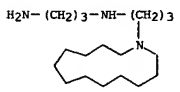
Double bond geometry as shown.



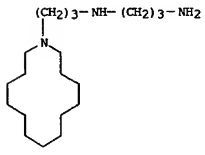
REFERENCE COUNT: 41 . . THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:883060 CAPLUS
DOCUMENT NUMBER: 137:185705
TITLE: Application of ring-closing metathesis to the synthesis of unsaturated 14-membered lactams and the marine alkaloids motuporamines A-C
AUTHOR(S): Goldring, William Peter Donald
CORPORATE SOURCE: Univ. of British Columbia, Vancouver, BC, Can.
SOURCE: (2000) 370 pp. Avail.: UMI, Order No. DANQ56551
From: Diss. Abstr. Int., B 2001, 61(12), 6477
DOCUMENT TYPE: Dissertation
LANGUAGE: English
AB Unavailable
IT **211566-77-7P**, Motuporamine A **211566-78-8P**, Motuporamine B **211569-34-5P**, Motuporamine C
RL: PNU (Preparation, unclassified); PREP (Preparation)
(application of ring-closing metathesis to synthesis of unsatd. 14-membered lactams and marine alkaloids motuporamines A-C)
RN 211566-77-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)



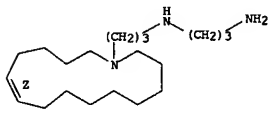
RN 211566-78-8 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)



RN 211569-34-5 CAPLUS
CN 1,3-Propanediamine, N-[3-[(6Z)-azacyclopentadec-6-en-1-yl]propyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L4 ANSWER 3 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

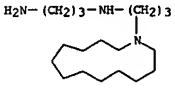


L4 ANSWER 4 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:712129 CAPLUS
DOCUMENT NUMBER: 136:63714
TITLE: Inhibition of tumor cell invasion and angiogenesis by motuporamines
AUTHOR(S): Roskelley, Calvin D.; Williams, David E.; McHardy, Lianne M.; Leong, Kevin G.; Trousdard, Armelle; Karsan, Aly; Andersen, Raymond J.; Dedhar, Shoukat; Roberge, Michel
CORPORATE SOURCE: Departments of Anotomy, University of British Columbia, Vancouver, BC, V6T 1Z3, Can.
SOURCE: Cancer Research (2001), 61(18), 6788-6794
CODEN: CNREA8; ISSN: 0008-5472
PUBLISHER: American Association for Cancer Research
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Tissue invasion is an important determinant of angiogenesis and metastasis and constitutes an attractive target for cancer therapy. We have developed an assay to identify agents that inhibit invasion by mechanisms other than inhibition of cell attachment or cytotoxicity. A screen of marine sponge exts. identified motuporamines as micromolar inhibitors of invasion of basement membrane gels by MDA-231 breast carcinoma, PC-3 prostate carcinoma, and U-87 and U-251 glioma cells. Motuporamine C inhibits cell migration in monolayer cultures and impairs actin-mediated membrane ruffling at the leading edge of lamellae. Motuporamine C also reduces .beta.1-integrin activation, raising the possibility that it interferes with "inside-out" signaling to integrins. In addn., motuporamine C inhibits angiogenesis in an in vitro sprouting assay with human endothelial cells and an in vivo chick chorioallantoic membrane assay. The motuporamines show little or no toxicity or inhibition of cell proliferation, and they are structurally simple and easy to synthesize, making them attractive drug candidates.

IT **211566-77-7**, Motuporamine A **211569-34-5**, Motuporamine C **251349-16-3** **385437-34-3**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(inhibition of tumor cell invasion and angiogenesis by motuporamines)

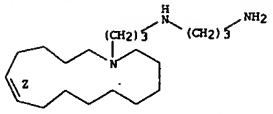
RN 211566-77-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)



RN 211569-34-5 CAPLUS
CN 1,3-Propanediamine, N-[3-[(6Z)-azacyclopentadec-6-en-1-yl]propyl]- (9CI) (CA INDEX NAME)

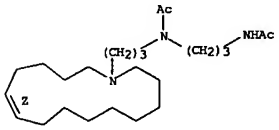
Double bond geometry as shown.

L4 ANSWER 4 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



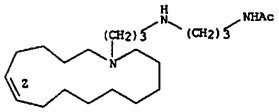
RN 251349-16-3 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



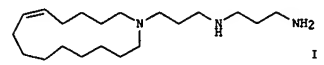
RN 385437-34-3 CAPLUS
CN Acetamide, N-[3-[[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]amino]propyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

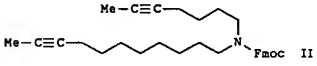


REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:191704 CAPLUS
DOCUMENT NUMBER: 133:43691
TITLE: Ring-Closing Alkyne Metathesis. Stereoselective Synthesis of the Cytotoxic Marine Alkaloid Motuporamine C
AUTHOR(S): Fuerstner, Alois; Rumbo, Antonio
CORPORATE SOURCE: Max-Planck-Institut fuer Kohlenforschung, Muelheim/Ruhr, D-45470, Germany
SOURCE: Journal of Organic Chemistry (2000), 65(8), 2608-2611
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:43691
GI



I



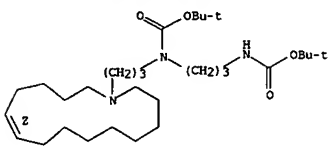
II

AB Motuporamine C (I) was synthesized from MeC.tplbond.C(CH2)8OH in 8 steps via ring-closing alkyne metathesis of the undecynylheptynylamine II followed by alkylation.

IT **274675-60-4P** **274675-68-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective synthesis of the cytotoxic marine alkaloid motuporamine C)

RN 274675-60-4 CAPLUS
CN Carbamic acid, [3-(6Z)-azacyclopentadec-6-en-1-ylpropyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

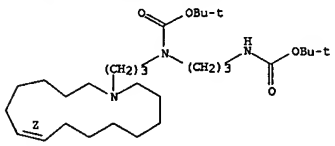
Double bond geometry as shown.



RN 274675-68-2 CAPLUS

L4 ANSWER 5 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
CN Carbamic acid, [3-(7Z)-azacyclopentadec-7-en-1-ylpropyl][3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

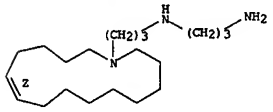
Double bond geometry as shown.



IT **211569-34-5P** **274675-53-5P** **274675-69-3P** **274675-70-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective synthesis of the cytotoxic marine alkaloid motuporamine C)

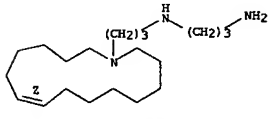
RN 211569-34-5 CAPLUS
CN 1,3-Propanediamine, N-[3-[(6Z)-azacyclopentadec-6-en-1-yl]propyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



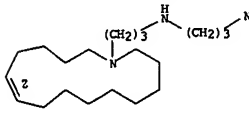
RN 274675-53-5 CAPLUS
CN 1,3-Propanediamine, N-[3-(7Z)-azacyclopentadec-7-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 274675-69-3 CAPLUS
CN 1,3-Propanediamine, N-[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]-, dihydrochloride (9CI) (CA INDEX NAME)

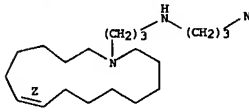
L4 ANSWER 5 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
Double bond geometry as shown.



●2 HCl

RN 274675-70-6 CAPLUS
CN 1,3-Propanediamine, N-[3-(7Z)-azacyclopentadec-7-en-1-ylpropyl]-, dihydrochloride (9CI) (CA INDEX NAME)

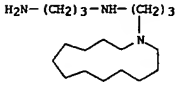
Double bond geometry as shown.



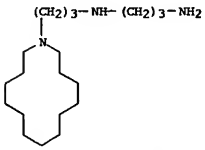
●2 HCl

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:715619 CAPLUS
DOCUMENT NUMBER: 132:122787
TITLE: Cytotoxic alkaloids motuporamines A-C, synthesis and structural verification. [Erratum to document cited in CA132:12426]
AUTHOR(S): Goldring, William P. D.; Weiler, Larry
CORPORATE SOURCE: Dep. Chemistry, Univ. British Columbia, Vancouver, BC, V6T 1Z1, Can.
SOURCE: Organic Letters (1999), 1(11), 1874
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The cor. ref. 2 should read as follows: "(2) Baldwin, J. E.; Vollmer, H. R.; Lee, V. Tetrahedron Lett. 1999, 40, 5401.".
IT **211566-77-7P**, Motuporamine A **211566-78-8P**, Motuporamine B **251349-24-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(cytotoxic alkaloids motuporamines A-C, synthesis and structural verification (Erratum))
RN 211566-77-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)

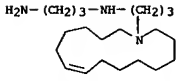


RN 211566-78-8 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)

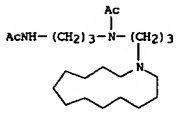


RN 251349-24-3 CAPLUS
CN 1,3-Propanediamine, N-[3-(azacyclopentadec-7-en-1-yl)propyl]- (9CI) (CA INDEX NAME)

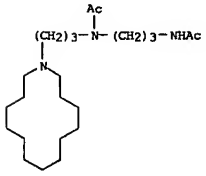
L4 ANSWER 6 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



IT **211388-13-5P 211388-14-6P 211569-34-5P**, Motuporamine C **251349-16-3P 251349-25-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(cytotoxic alkaloids motuporamines A-C, synthesis and structural verification (Erratum))
RN 211388-13-5 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)



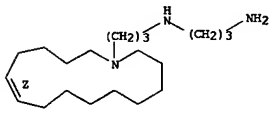
RN 211388-14-6 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)



RN 211569-34-5 CAPLUS
CN 1,3-Propanediamine, N-[3-[(6Z)-azacyclopentadec-6-en-1-yl]propyl]- (9CI) (CA INDEX NAME)

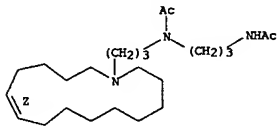
Double bond geometry as shown.

L4 ANSWER 6 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

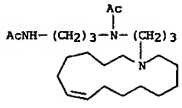


RN 251349-16-3 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

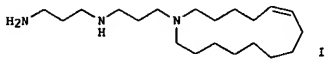
Double bond geometry as shown.



RN 251349-25-4 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(azacyclopentadec-7-en-1-yl)propyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 7 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:629478 CAPLUS
DOCUMENT NUMBER: 132:12426
TITLE: Cytotoxic Alkaloids Motuporamines A-C: Synthesis and Structural Verification
AUTHOR(S): Goldring, William P. D.; Weiler, Larry
CORPORATE SOURCE: Department of Chemistry, University of British Columbia, Vancouver, BC, V6T 1Z1, Can.
SOURCE: Organic Letters (1999), 1(9), 1471-1473
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:12426
GI

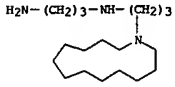


I

AB The unusual structure and biol. properties of the marine alkaloids motuporamines A-C, as well as the uncertainty as to the position of the olefin within the ring of motuporamine C, led to the synthesis of these compds. The strategy utilized the ring-closing metathesis reaction to form the 14- and 15-membered rings and Michael addn. and amidation chem. to introduce the spermine-like unit. The syntheses, structure assignment verifications, and also the detn. of the position of the olefin in motuporamine C (I) are described.

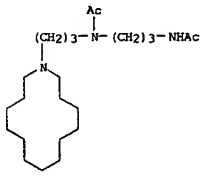
IT **211566-77-7P**, Motuporamine A **211566-78-8P**, Motuporamine B **251349-24-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(cytotoxic alkaloids motuporamines A-C, synthesis and structural verification)

RN 211566-77-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)



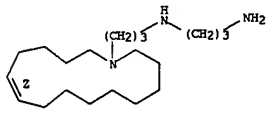
RN 211566-78-8 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 7 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



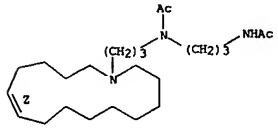
RN 211569-34-5 CAPLUS
CN 1,3-Propanediamine, N-[3-[(6Z)-azacyclopentadec-6-en-1-yl]propyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



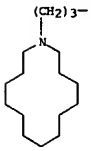
RN 251349-16-3 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(6Z)-azacyclopentadec-6-en-1-ylpropyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

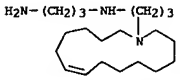


RN 251349-25-4 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(azacyclopentadec-7-en-1-yl)propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 7 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

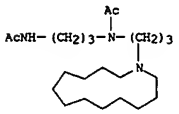


RN 251349-24-3 CAPLUS
CN 1,3-Propanediamine, N-[3-(azacyclopentadec-7-en-1-yl)propyl]- (9CI) (CA INDEX NAME)



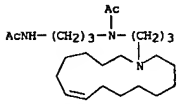
IT **211388-13-5P 211388-14-6P 211569-34-5P**, Motuporamine C **251349-16-3P 251349-25-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(cytotoxic alkaloids motuporamines A-C, synthesis and structural verification)

RN 211388-13-5 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)



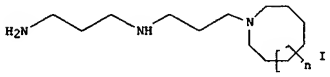
RN 211388-14-6 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 7 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

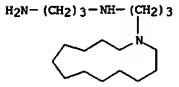


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:448471 CAPLUS
DOCUMENT NUMBER: 131:257741
TITLE: Total synthesis of cytotoxic sponge alkaloids motuporamines A and B
AUTHOR(S): Baldwin, Jack E.; Vollmer, Heidi R.; Lee, Victor
CORPORATE SOURCE: The Dyson Perrins Laboratory, University of Oxford, Oxford, OX1 3QY, UK
SOURCE: Tetrahedron Letters (1999), 40(29), 5401-5404
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:257741
GI

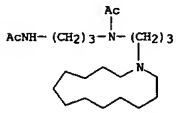


AB The synthesis of two sponge alkaloids, motuporamines A and B (I) (n = 6, 7) is reported. The key step involved a reductive amination using sodium triacetoxyborohydride.
IT **211566-77-7P 211566-78-8P 245119-67-9P**
245119-68-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(total synthesis of cytotoxic sponge alkaloids motuporamines A and B)
RN 211566-77-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)

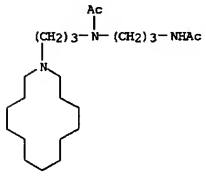


RN 211566-78-8 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 8 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
(total synthesis of cytotoxic sponge alkaloids motuporamines A and B)
RN 211388-13-5 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)

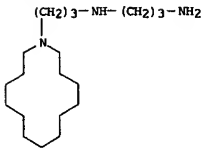


RN 211388-14-6 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)

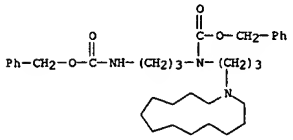


REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

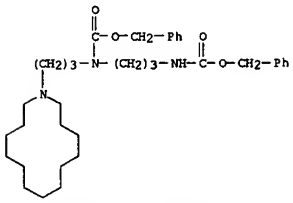
L4 ANSWER 8 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



RN 245119-67-9 CAPLUS
CN Carbamic acid, (3-azacyclotridec-1-ylpropyl)[3-[[(phenylmethoxy)carbonyl]amino]propyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

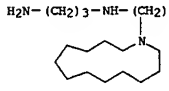


RN 245119-68-0 CAPLUS
CN Carbamic acid, (3-azacyclotetradec-1-ylpropyl)[3-[[(phenylmethoxy)carbonyl]amino]propyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

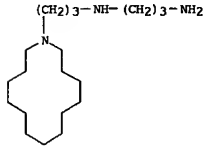


IT **211388-13-5P 211388-14-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)

L4 ANSWER 9 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1998:446771 CAPLUS
DOCUMENT NUMBER: 129:173061
TITLE: Motuporamines A-C, Cytotoxic Alkaloids Isolated from the Marine Sponge Xestospongia exigua (Kirkpatrick)
AUTHOR(S): Williams, David E.; Lassota, Peter; Andersen, Raymond J.
CORPORATE SOURCE: Departments of Chemistry and Oceanography Earth Ocean Sciences, University of British Columbia, Vancouver, BC, V6T 1Z1, Can.
SOURCE: Journal of Organic Chemistry (1998), 63(14), 4838-4841
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Bioassay guided fractionation of the Xestospongia exigua exts. yielded a mixt. of motuporamines A-C, which contain a spermidine-like substructure and represent a new family of cytotoxic sponge alkaloids. The motuporamines A-C were diacetylated and sepd. via reversed phase HPLC. NMR data for the motuporamines and their diacetates was detailed.
IT **211566-77-7P**, Motuporamine A **211566-78-8P**, Motuporamine B **211569-34-5P**, Motuporamine C
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(isolation of motuporamines A-C, cytotoxic alkaloids, from the marine sponge Xestospongia exigua)
RN 211566-77-7 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotridec-1-ylpropyl)- (9CI) (CA INDEX NAME)



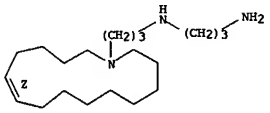
RN 211566-78-8 CAPLUS
CN 1,3-Propanediamine, N-(3-azacyclotetradec-1-ylpropyl)- (9CI) (CA INDEX NAME)



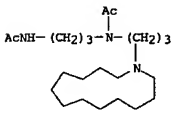
RN 211569-34-5 CAPLUS
CN 1,3-Propanediamine, N-[3-[(6Z)-azacyclopentadec-6-en-1-yl]propyl]- (9CI)

L4 ANSWER 9 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
(CA INDEX NAME)

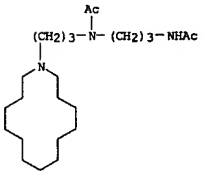
Double bond geometry as shown.



IT **211388-13-5P**, Diacetylmotuporamine A **211388-14-6P**,
Diacetylmotuporamine B **251349-16-3P**, Diacetylmotuporamine C
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(isolation of motuporamines A-C, cytotoxic alkaloids, from the marine sponge Xestospongia exigua)
RN 211388-13-5 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-(3-azacyclotridec-1-ylpropyl)-
(9CI) (CA INDEX NAME)



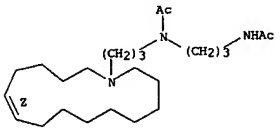
RN 211388-14-6 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-(3-azacyclotetradec-1-ylpropyl)-
(9CI) (CA INDEX NAME)



RN 251349-16-3 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-(62)-azacyclopentadec-6-en-1-

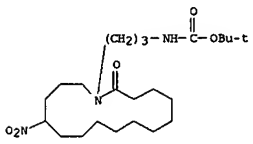
L4 ANSWER 9 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
ylpropyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

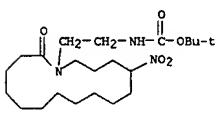


REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1994:77488 CAPLUS
DOCUMENT NUMBER: 120:77488
TITLE: The mass spectral loss of water from macrocyclic amino ketones
AUTHOR(S): Benz, Herbert; Hesse, Manfred
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, CH-8057, Switz.
SOURCE: Helvetica Chimica Acta (1993), 76(4), 1636-48
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
AB Macrocyclic oxo-lactams contg. an aminoalkyl side chain are stable natural products. Their electron-impact mass spectra are characterized by intense [M - H2O]+ signals, the mol. ion signal itself is missing. Under electrospray ionization conditions, on the other hand, the [M + 1]+ ion is the only detected signal. The loss of water is explained in terms of an internal (thermal) Schiff-base formation, leading to, e.g., a bicyclo[11.9.4]-system. The alcs. corresponding to the macrocyclic ketones and/or lactams show expected mass-spectral behavior following well-known rules.
IT **99379-76-7P 152450-40-3P 152450-42-5P**
152450-43-6P 152450-44-7P 152450-45-8P
152450-46-9P 152450-47-0P 152450-48-1P
152450-49-2P 152450-50-5P 152450-51-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(intermediate in prepn. of aminoalkyl macrocyclic lactams)
RN 99379-76-7 CAPLUS
CN Carbamic acid, [3-(13-nitro-2-oxoazacyclohexadec-1-yl)propyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

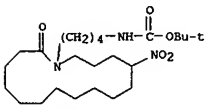


RN 152450-40-3 CAPLUS
CN Carbamic acid, [2-(13-nitro-2-oxoazacyclohexadec-1-yl)ethyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

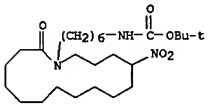


RN 152450-42-5 CAPLUS
CN Carbamic acid, [4-(13-nitro-2-oxoazacyclohexadec-1-yl)butyl]-,

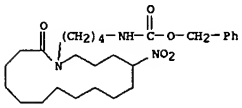
L4 ANSWER 10 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



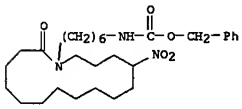
RN 152450-43-6 CAPLUS
CN Carbamic acid, [6-(13-nitro-2-oxoazacyclohexadec-1-yl)hexyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 152450-44-7 CAPLUS
CN Carbamic acid, [4-(13-nitro-2-oxoazacyclohexadec-1-yl)butyl]-,
phenylmethyl ester (9CI) (CA INDEX NAME)

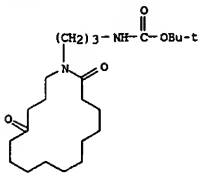


RN 152450-45-8 CAPLUS
CN Carbamic acid, [6-(13-nitro-2-oxoazacyclohexadec-1-yl)hexyl]-,
phenylmethyl ester (9CI) (CA INDEX NAME)

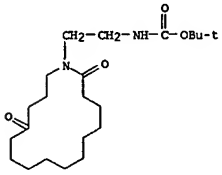


RN 152450-46-9 CAPLUS
CN Carbamic acid, [3-(2,13-dioxoazacyclohexadec-1-yl)propyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

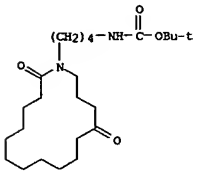
L4 ANSWER 10 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



RN 152450-47-0 CAPLUS
CN Carbamic acid, [2-(2,13-dioxoazacyclohexadec-1-yl)ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

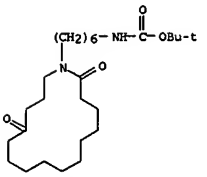


RN 152450-48-1 CAPLUS
CN Carbamic acid, [4-(2,13-dioxoazacyclohexadec-1-yl)butyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

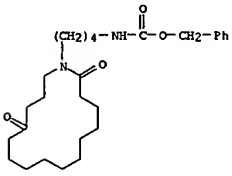


RN 152450-49-2 CAPLUS
CN Carbamic acid, [6-(2,13-dioxoazacyclohexadec-1-yl)hexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

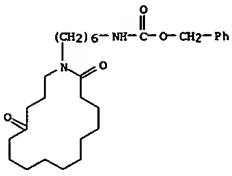
L4 ANSWER 10 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



RN 152450-50-5 CAPLUS
CN Carbamic acid, [4-(2,13-dioxoazacyclohexadec-1-yl)butyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

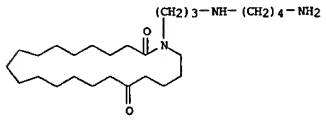


RN 152450-51-6 CAPLUS
CN Carbamic acid, [6-(2,13-dioxoazacyclohexadec-1-yl)hexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

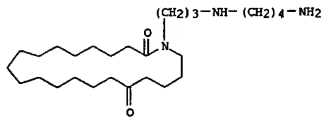


IT **152450-26-5**

L4 ANSWER 10 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
RL: PRP (Properties)
(mass spectrum of)
RN 152450-26-5 CAPLUS
CN Azacycloheneicosane-2,17-dione, 1-[3-[(4-aminobutyl)amino]propyl]- (9CI) (CA INDEX NAME)

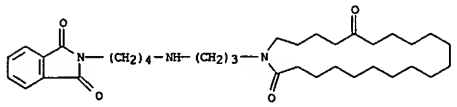


IT **152450-23-2 152450-24-3 152450-25-4 152450-29-8 152450-32-3 152450-34-5 152450-35-6**
RL: PRP (Properties)
(mass spectrum of, water loss in)
RN 152450-23-2 CAPLUS
CN Azacycloheneicosane-2,17-dione, 1-[3-[(4-aminobutyl)amino]propyl]-, dihydrochloride (9CI) (CA INDEX NAME)



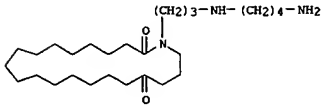
●2 HCl

RN 152450-24-3 CAPLUS
CN 1H-Isoindole-1,3(2H)-dione, 2-[4-[[3-(2,17-dioxoazacycloheneicos-1-yl)propyl]amino]butyl]-, monohydrochloride (9CI) (CA INDEX NAME)



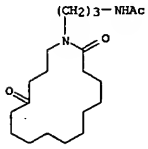
● HCl

L4 ANSWER 10 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
RN 152450-25-4 CAPLUS
CN Azacycloheneicosane-2,18-dione, 1-[3-[(4-aminobutyl)amino]propyl]-, dihydrochloride (9CI) (CA INDEX NAME)

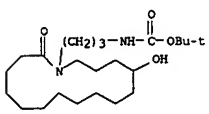


●2 HCl

RN 152450-29-8 CAPLUS
CN Acetamide, N-[3-(2,13-dioxoazacyclohexadec-1-yl)propyl]- (9CI) (CA INDEX NAME)

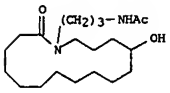


RN 152450-32-3 CAPLUS
CN Carbamic acid, [3-(13-hydroxy-2-oxoazacyclohexadec-1-yl)propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

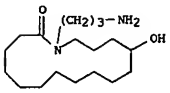


RN 152450-34-5 CAPLUS
CN Acetamide, N-[3-(13-hydroxy-2-oxoazacyclohexadec-1-yl)propyl]- (9CI) (CA INDEX NAME)

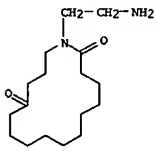
L4 ANSWER 10 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



RN 152450-35-6 CAPLUS
CN Azacyclohexadecan-2-one, 1-(3-aminopropyl)-13-hydroxy- (9CI) (CA INDEX NAME)

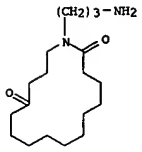


IT **152450-27-6P 152450-28-7P 152450-30-1P 152450-31-2P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and mass spectrum of, water loss in)
RN 152450-27-6 CAPLUS
CN Azacyclohexadecane-2,13-dione, 1-(2-aminoethyl)- (9CI) (CA INDEX NAME)

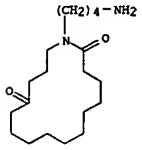


RN 152450-28-7 CAPLUS
CN Azacyclohexadecane-2,13-dione, 1-(3-aminopropyl)- (9CI) (CA INDEX NAME)

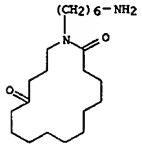
L4 ANSWER 10 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



RN 152450-30-1 CAPLUS
CN Azacyclohexadecane-2,13-dione, 1-(4-aminobutyl)- (9CI) (CA INDEX NAME)

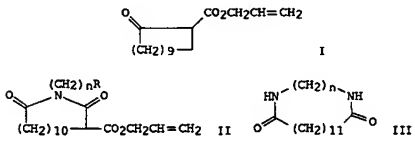


RN 152450-31-2 CAPLUS
CN Azacyclohexadecane-2,13-dione, 1-(6-aminohexyl)- (9CI) (CA INDEX NAME)



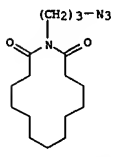
L4 ANSWER 11 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1992:174126 CAPLUS
DOCUMENT NUMBER: 116:174126
TITLE: Synthesis of macrocycles by ring enlargement of 14-membered cyclic imides
AUTHOR(S): Koch, Thomas; Ognyanov, Vassil I.; Hesse, Manfred
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, CH-8057, Switz.
SOURCE: Helvetica Chimica Acta (1992), 75(1), 62-8
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 116:174126
GI



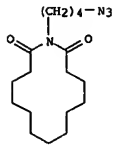
AB In the presence of a base, cyclododecanone deriv. I, activated in .alpha.-position by the allyloxycarbonyl group, underwent ring enlargement with isocyanates to give 14-membered imides II (n = 3, R = Cl; n = 4, R = Br). Cleavage of the activating group gave new 14-membered imides which were transformed by further ring-enlargement reactions into the new macrocyclic compds. III.

IT **139662-47-8P 139662-48-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and transamidation of)
RN 139662-47-8 CAPLUS
CN Azacyclotetradecane-2,14-dione, 1-(3-azidopropyl)- (9CI) (CA INDEX NAME)



RN 139662-48-9 CAPLUS
CN Azacyclotetradecane-2,14-dione, 1-(4-azidobutyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 11 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

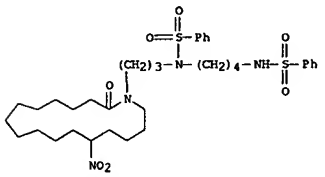


L4 ANSWER 12 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1989:554188 CAPLUS
DOCUMENT NUMBER: 111:154188
TITLE: Syntheses of the spermidine alkaloids (.+-.)-inandenin-10-ol, inandenin-10-one, and (.+-.)-oncinotine
AUTHOR(S): Bienz, Stefan; Guggisberg, Armin; Waelchli, Rudolf; Hesse, Manfred
CORPORATE SOURCE: Org. Chem. Inst., Univ. Zurich, Zurich, CH-8057, Switz.
SOURCE: Helvetica Chimica Acta (1988), 71(7), 1708-18
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 111:154188
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

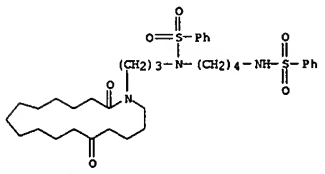
AB (.+-.)-Inandenin-10-ol (I, X = H,HO), inandenin-10-one (I, X = O) and (.+-.)-oncinotine (II) were prepd. from the aldehyde III and PhSO2NH(CH2)4N(SO2Ph)(CH2)3NH2 via ring expansion of the dodecanone deriv. IV and transamidation of the lactam V.

IT 122890-18-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and Neff reaction of)
RN 122890-18-0 CAPLUS
CN Benzenesulfonamide, N-[3-(13-nitro-2-oxoazacycloheptadec-1-yl)propyl]-N-[4-[(phenylsulfonyl)amino]butyl]- (9CI) (CA INDEX NAME)

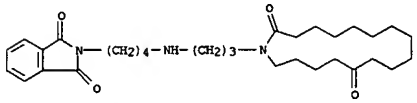


IT 122890-28-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and chlorination of)
RN 122890-28-2 CAPLUS
CN 1H-Isoindole-1,3(2H)-dione, 2-[4-[[3-(13-hydroxy-2-oxoazacycloheptadec-1-yl)propyl]amino]butyl]-, monohydrochloride (9CI) (CA INDEX NAME)

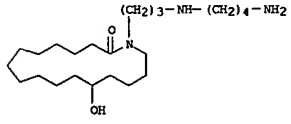
L4 ANSWER 12 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



IT 122890-27-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and intramol. cyclization of)
RN 122890-27-1 CAPLUS
CN Azacycloheptadecane-2,13-dione, 1-[3-[[4-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)butyl]amino]propyl]- (9CI) (CA INDEX NAME)



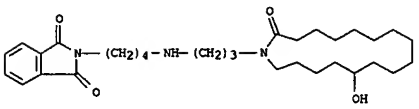
IT 122890-20-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and ring expansion of)
RN 122890-20-4 CAPLUS
CN Azacycloheptadecan-2-one, 1-[3-[[4-aminobutyl)amino]propyl]-13-hydroxy-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

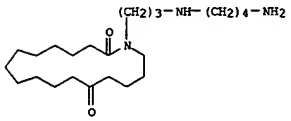
IT 122890-23-7P 122890-24-8P 122890-29-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L4 ANSWER 12 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



● HCl

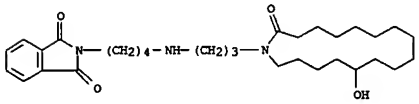
IT 122890-26-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conversion to phthalimido deriv.)
RN 122890-26-0 CAPLUS
CN Azacycloheptadecane-2,13-dione, 1-[3-[(4-aminobutyl)amino]propyl]-, dihydrochloride (9CI) (CA INDEX NAME)



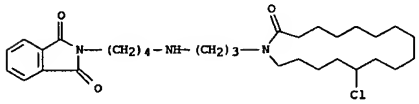
●2 HCl

IT 122890-19-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and electrochem. redn. of)
RN 122890-19-1 CAPLUS
CN Benzenesulfonamide, N-[3-(2,13-dioxoazacycloheptadec-1-yl)propyl]-N-[4-[(phenylsulfonyl)amino]butyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 12 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
RN 122890-23-7 CAPLUS
CN 1H-Isoindole-1,3(2H)-dione, 2-[4-[[3-(13-hydroxy-2-oxoazacycloheptadec-1-yl)propyl]amino]butyl]- (9CI) (CA INDEX NAME)

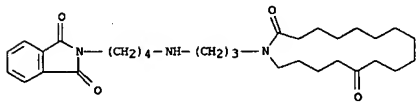


RN 122890-24-8 CAPLUS
CN 1H-Isoindole-1,3(2H)-dione, 2-[4-[[3-(13-chloro-2-oxoazacycloheptadec-1-yl)propyl]amino]butyl]-, monohydrochloride (9CI) (CA INDEX NAME)



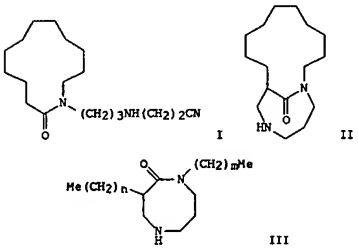
● HCl

RN 122890-29-3 CAPLUS
CN Azacycloheptadecane-2,13-dione, 1-[3-[[4-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)butyl]amino]propyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

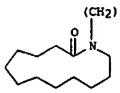
L4 ANSWER 13 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1986:5757 CAPLUS
DOCUMENT NUMBER: 104:5757
TITLE: Transamidation reactions. Part 11. N-Substituted 3-aminopropanenitriles and 2-aminoacetonitriles as Schiff-base equivalents
AUTHOR(S): Askitoglu, Elefteria; Guggisberg, Armin; Hesse, Manfred
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, CH-8057, Switz.
SOURCE: Helvetica Chimica Acta (1985), 68(3), 750-9
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 104:5757
GI



AB Treating (oxoazacyclotridecyl)azaheptanenitrile I with KNH(CH2)3NH2-NH2(CH2)3NH2 or with Me3COK-PhMe gave the unexpected bicyclic product II. Similarly, treatment of Me(CH2)nCH2CON[(CH2)mMe](CH2)3NH(CH2)6CN (n = m = 0; n = 4, m = 5) with Me3COK-PhMe gave the diazacyclooctanones III. The reaction proceeds via an intermediate formaldehyde imine.

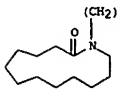
IT 99014-99-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of)
RN 99014-99-0 CAPLUS
CN Propanenitrile, 3-[[3-(2-oxoazacyclotridec-1-yl)propyl]amino]-, monohydrochloride (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

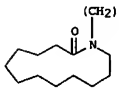


● HCl

IT 67171-82-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, in presence of strong base)
RN 67171-82-8 CAPLUS
CN Propanenitrile, 3-[[3-(2-oxoazacyclotridec-1-yl)propyl]amino]- (9CI) (CA INDEX NAME)

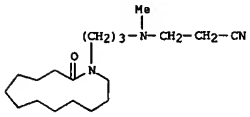


IT 99014-95-6P 99014-96-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and cyclization of)
RN 99014-95-6 CAPLUS
CN Acetonitrile, [[3-(2-oxoazacyclotridec-1-yl)propyl]amino]- (9CI) (CA INDEX NAME)

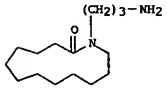


RN 99014-96-7 CAPLUS
CN Propanenitrile, 3-[methyl[3-(2-oxoazacyclotridec-1-yl)propyl]amino]- (9CI) (CA INDEX NAME)

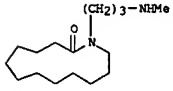
L4 ANSWER 13 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



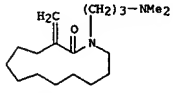
IT 64414-61-5P 67370-86-9P 99014-86-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 64414-61-5 CAPLUS
CN Azacyclotridecan-2-one, 1-(3-aminopropyl)- (9CI) (CA INDEX NAME)



RN 67370-86-9 CAPLUS
CN Azacyclotridecan-2-one, 1-[3-(methylamino)propyl]- (9CI) (CA INDEX NAME)

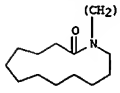


RN 99014-86-5 CAPLUS
CN Azacyclotridecan-2-one, 1-[3-(dimethylamino)propyl]-3-methylene- (9CI) (CA INDEX NAME)



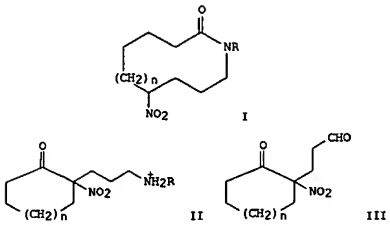
IT 99014-94-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactions of)
RN 99014-94-5 CAPLUS
CN Azacyclotridecan-2-one, 1-(3-aminopropyl)-, monohydrochloride (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



● HCl

L4 ANSWER 14 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1986:5756 CAPLUS
DOCUMENT NUMBER: 104:5756
TITLE: Synthesis of macrocyclic lactams from ketones by ring enlargement reaction
AUTHOR(S): Waelchli, Rudolf; Bienz, Stefan; Hesse, Manfred
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, CH-8057, Switz.
SOURCE: Helvetica Chimica Acta (1985), 68(2), 484-92
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 104:5756
GI

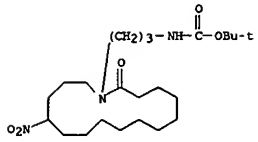


AB The macrocyclic lactams I [R = PhCH2, n = 1, 3, 7; R = Pr, n = 3, 7; R = Me(CH2)4, Me3C, HO(CH2)3, Me3CO2CNH(CH2)3, n = 7] were prepd. by ring expansion of the (aminopropyl)nitrocycloalkanones II by treatment with NaHCO3 in H2O/MeOH. II were prepd. by reductive amination of the aldehydes III.

IT **99379-76-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 99379-76-7 CAPLUS
CN Carbamic acid, [3-(13-nitro-2-oxoazacyclohexadec-1-yl)propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 14 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



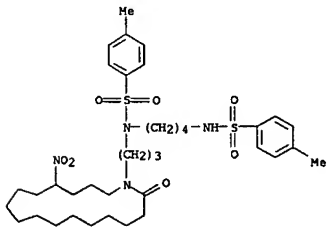
L4 ANSWER 15 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1985:221067 CAPLUS
DOCUMENT NUMBER: 102:221067
TITLE: Synthesis of N-(4-aminobutyl)-16-aza-19-nonadecane lactam and N-(4-aminobutyl)-17-aza-20-icosane lactam (deoxoinandenine)
AUTHOR(S): Waelchli, Rudolf; Guggisberg, Armin; Hesse, Manfred
CORPORATE SOURCE: Org. Chem. Inst., Univ. Zurich, Zurich, CH-8057, Switz.
SOURCE: Helvetica Chimica Acta (1984), 67(8), 2178-85
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I (n = 1, 0) were prepd. from cyclotridecanone and cyclododecanone, resp. via ring enlargement of the aminopropyl cycloalkanone derivs. II and III.

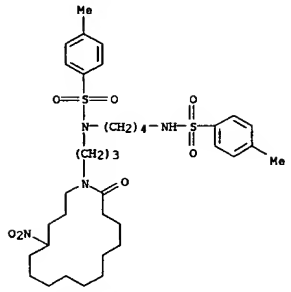
IT **91653-21-3P 96624-95-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conversion to ketone)

RN 91653-21-3 CAPLUS
CN Benzenesulfonamide, 4-methyl-N-[4-[[(4-methylphenyl)sulfonyl]amino]butyl]-N-[3-(14-nitro-2-oxoazacycloheptadec-1-yl)propyl]- (9CI) (CA INDEX NAME)



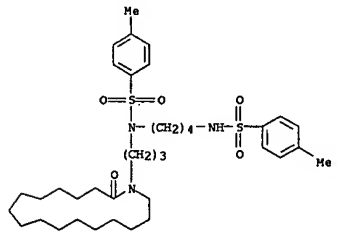
RN 96624-95-2 CAPLUS
CN Benzenesulfonamide, 4-methyl-N-[4-[[(4-methylphenyl)sulfonyl]amino]butyl]-N-[3-(13-nitro-2-oxoazacyclohexadec-1-yl)propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



IT **91652-54-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and detolsylation of)

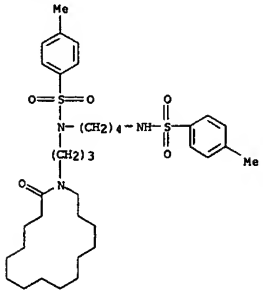
RN 91652-54-9 CAPLUS
CN Benzenesulfonamide, 4-methyl-N-[4-[[(4-methylphenyl)sulfonyl]amino]butyl]-N-[3-(2-oxoazacycloheptadec-1-yl)propyl]- (9CI) (CA INDEX NAME)



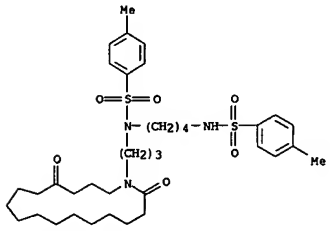
IT **96624-97-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and detosylation of)

RN 96624-97-4 CAPLUS
CN Benzenesulfonamide, 4-methyl-N-[4-[[(4-methylphenyl)sulfonyl]amino]butyl]-N-[3-(2-oxoazacyclohexadec-1-yl)propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

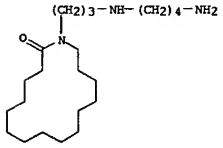


IT **91652-53-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and ketalization of ethylenedithiol)
RN 91652-53-8 CAPLUS
CN Benzenesulfonamide, N-[3-(2,14-dioxoazacycloheptadec-1-yl)propyl]-4-methyl-N-[4-[[(4-methylphenyl)sulfonyl]amino]butyl]- (9CI) (CA INDEX NAME)

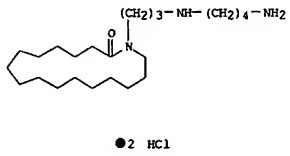


IT **96624-96-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and ketalization with ethanedithiol)
RN 96624-96-3 CAPLUS
CN Benzenesulfonamide, N-[3-(2,13-dioxoazacyclohexadec-1-yl)propyl]-4-methyl-N-[4-[[(4-methylphenyl)sulfonyl]amino]butyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 15 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

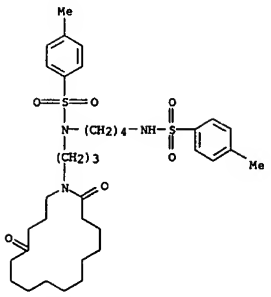


IT **96624-98-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 96624-98-5 CAPLUS
CN Azacycloheptadecan-2-one, 1-[3-[(4-aminobutyl)amino]propyl]-, dihydrochloride (9CI) (CA INDEX NAME)

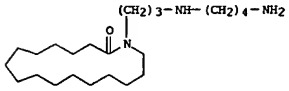


●2 HCl

L4 ANSWER 15 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

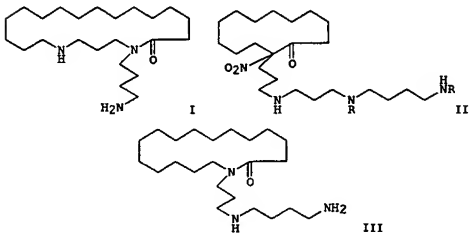


IT **91653-20-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and ring enlargement of, (aminobutyl)azaicosane lactam from)
RN 91653-20-2 CAPLUS
CN Azacycloheptadecan-2-one, 1-[3-[(4-aminobutyl)amino]propyl]- (9CI) (CA INDEX NAME)



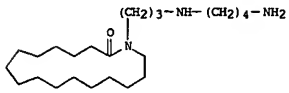
IT **96624-94-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and ring enlargement of, (aminobutyl)azanondecane lactam from)
RN 96624-94-1 CAPLUS
CN Azacyclohexadecan-2-one, 1-[3-[(4-aminobutyl)amino]propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 16 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1984:511239 CAPLUS
DOCUMENT NUMBER: 101:111239
TITLE: Ring expansion reactions in the formation of macrocyclic lactams. A synthesis of deoxoinandenine
AUTHOR(S): Waelchli, Rudolf; Guggisberg, Armin; Hesse, Manfred
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zuerich, Zurich, CH-8057, Switz.
SOURCE: Tetrahedron Letters (1984), 25(21), 2205-8
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



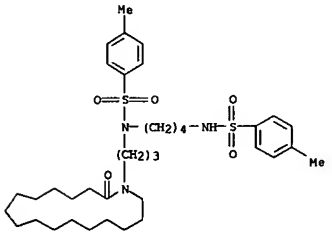
AB Deoxoinandenine (I), a redn. product of the macrocyclic spermidine alkaloids inandenin-12-one and -13-one was synthesized starting from 2-nitrocyclotridecanone by ring expansion reactions of macrocycles II (R = p-MeC6H4SO2) and III.

IT **91653-20-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and Zip ring expansion of)
RN 91653-20-2 CAPLUS
CN Azacycloheptadecan-2-one, 1-[3-[(4-aminobutyl)amino]propyl]- (9CI) (CA INDEX NAME)

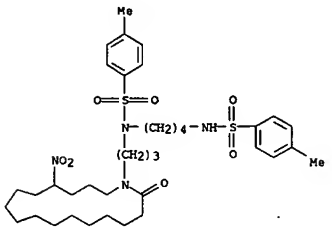


IT **91652-54-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and detosylation of)

L4 ANSWER 16 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
RN 91652-54-9 CAPLUS
CN Benzenesulfonamide, 4-methyl-N-[4-[[(4-methylphenyl)sulfonyl]amino]butyl]-N-[3-(2-oxoazacycloheptadec-1-yl)propyl]- (9CI) (CA INDEX NAME)

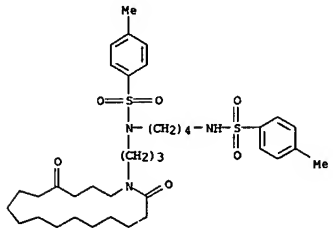


IT **91653-21-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and hydrolysis of)
RN 91653-21-3 CAPLUS
CN Benzenesulfonamide, 4-methyl-N-[4-[[(4-methylphenyl)sulfonyl]amino]butyl]-N-[3-(14-nitro-2-oxoazacycloheptadec-1-yl)propyl]- (9CI) (CA INDEX NAME)

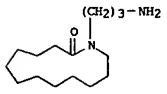


IT **91652-53-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and redn. of)
RN 91652-53-8 CAPLUS

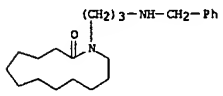
L4 ANSWER 16 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
CN Benzenesulfonamide, N-[3-(2,14-dioxoazacycloheptadec-1-yl)propyl]-4-methyl-N-[4-[[(4-methylphenyl)sulfonyl]amino]butyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 17 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1981:496437 CAPLUS
DOCUMENT NUMBER: 95:96437
TITLE: Transamidation reactions. Part 9. Amidines as intermediates in transamidation reactions
AUTHOR(S): Heidelberger, Christian; Guggisberg, Armin; Stephanou, Euripides; Hesse, Manfred
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, CH-8057, Switz.
SOURCE: Helvetica Chimica Acta (1981), 64(2), 399-406
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB Refluxing N-(aminoalkyl) lactams in xylene contg. p-MeC6H4SO3H gave bicyclic amidines, which were partially hydrolyzed in aq. KOH to give the starting and a ring-enlarged lactam. An example was the conversion of I to II, followed by hydrolysis to give I and III. N-[(Alkylamino)alkyl] lactams follow an analogous course via amidinium salts; e.g., IV was converted to V, which was hydrolyzed to give IV and VI. In some cases only 1 of the 2 isomeric lactams was formed in the alk. hydrolysis step.
IT **64414-61-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, amidine formation in)
RN 64414-61-5 CAPLUS
CN Azacyclotridecan-2-one, 1-(3-aminopropyl)- (9CI) (CA INDEX NAME)

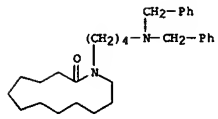


IT **72636-84-1 78097-27-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(ring enlargement of, in transamidation)
RN 72636-84-1 CAPLUS
CN Azacyclotridecan-2-one, 1-[3-[(phenylmethyl)amino]propyl]- (9CI) (CA INDEX NAME)



RN 78097-27-5 CAPLUS
CN Azacyclotridecan-2-one, 1-[4-[bis(phenylmethyl)amino]butyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 17 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



L4 ANSWER 18 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1980:128882 CAPLUS
DOCUMENT NUMBER: 92:128882
TITLE: Transamidation reactions. Part 8. Use of the 'Zip' reaction for the synthesis of a 53-membered polyamino lactam
AUTHOR(S): Kramer, Urs; Guggisberg, Armin; Hesse, Manfred
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, CH-8057, Switz.
SOURCE: Helvetica Chimica Acta (1979), 62(7), 2317-24
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The lactam I reacted with K 3-aminopropylamide/1,3-diaminopropane (Zip reaction) to give the 53-membered lactam II. I was prepd. in 8 steps from III and PhNH[(CH2)2N(TOS)]3(CH2)3I (TOS = tosyl).

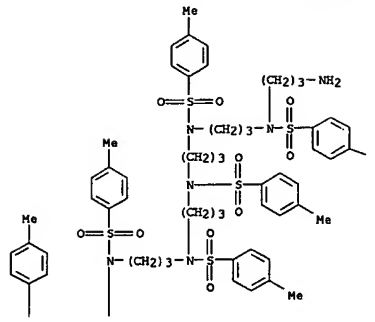
IT **73100-38-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and benzylation of)

RN 73100-38-6 CAPLUS

CN Benzenesulfonamide, N-[19-amino-4,8,12,16-tetrakis[(4-methylphenyl)sulfonyl]-4,8,12,16-tetraazanonadec-1-yl]-4-methyl-N-[4,8,12,16-tetrakis[(4-methylphenyl)sulfonyl]-19-(2-oxoazacyclotridec-1-yl)-4,8,12,16-tetraazanonadec-1-yl]-, monohydrochloride (9CI) (CA INDEX NAME)

L4 ANSWER 18 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 1-A



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L4 ANSWER 18 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

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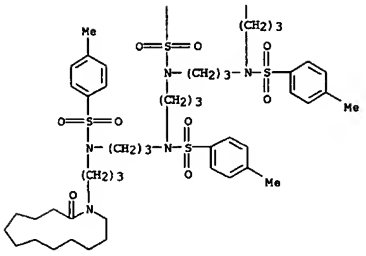


PAGE 2-B

● HCl

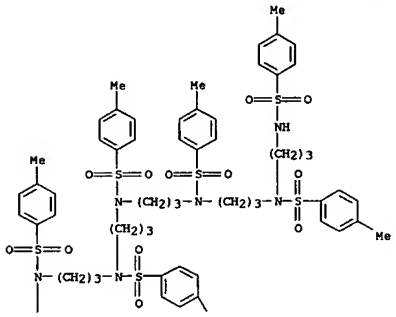
IT **65605-32-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and chain lengthening of)

RN 65605-32-5 CAPLUS

CN Benzenesulfonamide, 4-methyl-N-[3-[[(4-methylphenyl)sulfonyl][3-[[(4-methylphenyl)sulfonyl]amino]propyl]amino]propyl]-N-[3-[[(4-methylphenyl)sulfonyl][3-[[(4-methylphenyl)sulfonyl][3-[[(4-methylphenyl)sulfonyl][3-[(2-oxoazacyclotridec-1-yl)amino]propyl]amino]propyl]amino]propyl]amino]propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 18 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 1-A



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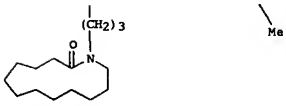

IT **65605-33-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and electrolysis of)

RN 65605-33-6 CAPLUS

CN Benzenesulfonamide, 4-methyl-N-[4,8,12,16-tetrakis[(4-methylphenyl)sulfonyl]-19-(2-oxoazacyclotridec-1-yl)-4,8,12,16-tetraazanonadec-1-yl]-N-[4,8,12,16-tetrakis[(4-methylphenyl)sulfonyl]-21-phenyl-20-(phenylmethyl)-4,8,12,16,20-pentaazaheneicos-1-yl]- (9CI) (CA INDEX NAME)

L4 ANSWER 18 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

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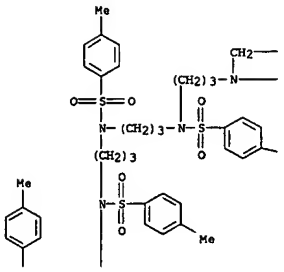

PAGE 1-B

—— Ph

—CH_2—Ph

L4 ANSWER 18 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

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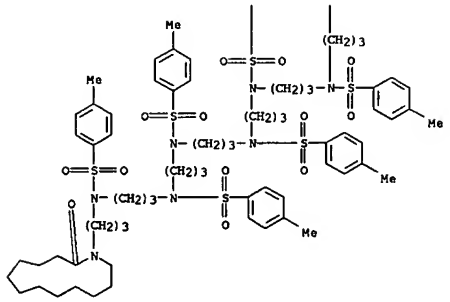

IT 73100-39-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and hydrogenolysis of)
RN 73100-39-7 CAPLUS
CN Azacyclotridecan-2-one, 1-[41-phenyl-40-(phenylmethyl)-4,8,12,16,20,24,28,32,36-nonaazahentetracont-1-yl]- (9CI) (CA INDEX NAME)

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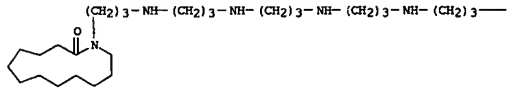

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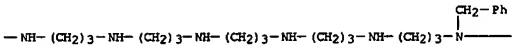

L4 ANSWER 18 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

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—CH_2—Ph

IT 73100-35-3P 73100-37-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with hydrazine)
RN 73100-35-3 CAPLUS
CN Benzenesulfonamide, N-[3-[[3-[[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propyl][(4-methylphenyl)sulfonyl]amino]propyl][(4-methylphenyl)sulfonyl]amino]propyl]-4-methyl-N-[3-[[(4-methylphenyl)sulfonyl][3-[[(4-methylphenyl)sulfonyl][3-(2-oxoazacyclotridec-1-yl)propyl]amino]propyl]amino]propyl]- (9CI) (CA INDEX NAME)

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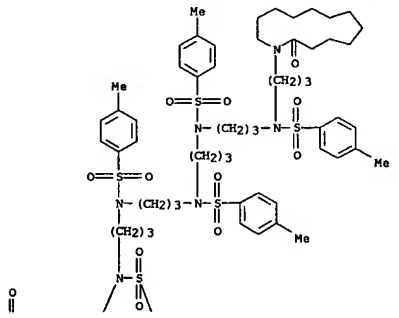

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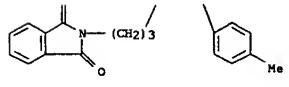

RN 73100-37-5 CAPLUS

L4 ANSWER 18 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

CN Benzenesulfonamide, N-[19-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)-4,8,12,16-tetrakis[(4-methylphenyl)sulfonyl]-4,8,12,16-tetraazanonadec-1-yl]-4-methyl-N-[4,8,12,16-tetrakis[(4-methylphenyl)sulfonyl]-19-(2-oxoazacyclotridec-1-yl)-4,8,12,16-tetraazanonadec-1-yl]- (9CI) (CA INDEX NAME)

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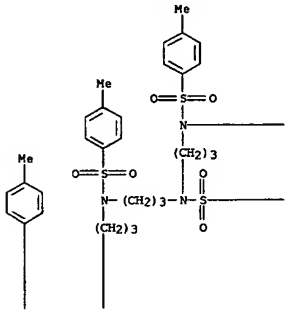

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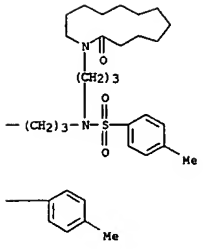

L4 ANSWER 18 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

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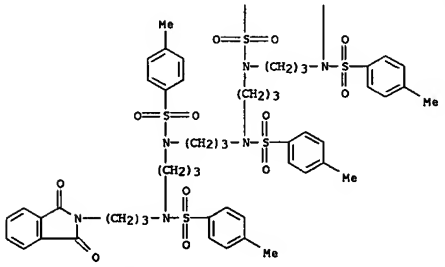

IT **65605-34-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and ring expansion of)
RN 65605-34-7 CAPLUS
CN Azacyclotridecan-2-one, 1-(39-amino-4,8,12,16,20,24,28,32,36-nonaazanonatriacont-1-yl)- (9CI) (CA INDEX NAME)

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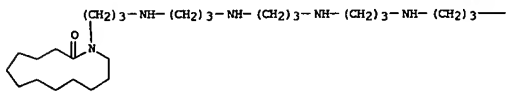

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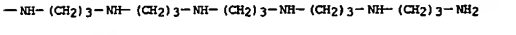

IT **73100-36-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and tosylation of)
RN 73100-36-4 CAPLUS
CN Benzenesulfonamide, N-[3-[[3-[(3-aminopropyl)[(4-methylphenyl)sulfonyl]amino]propyl][(4-methylphenyl)sulfonyl]amino]propyl]-4-methyl-N-[3-[[(4-methylphenyl)sulfonyl][3-[[(4-methylphenyl)sulfonyl][3-

L4 ANSWER 18 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

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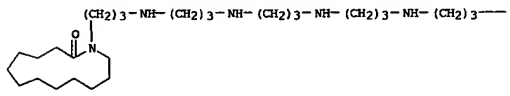

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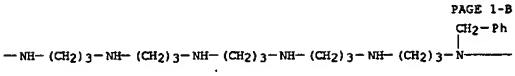
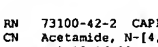


PAGE 1-C



RN 73100-42-2 CAPLUS
CN Acetamide, N-[4,8,12,16,20-pentaacetyl-23-(2-oxoazacyclotridec-1-yl)-4,8,12,16,20-pentaazatricos-1-yl]-N-(4,8,12-triacetyl-17-oxo-4,8,12,16-tetraazaoctadec-1-yl)- (9CI) (CA INDEX NAME)

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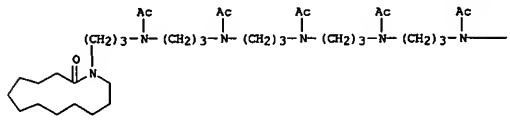
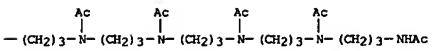


PAGE 1-B



IT **65545-59-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with iodopropyltripropylenetetramine deriv.)
RN 65545-59-7 CAPLUS

L4 ANSWER 18 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
(2-oxoazacyclotridec-1-yl)propyl]amino]propyl]amino]propyl]- (9CI) (CA INDEX NAME)

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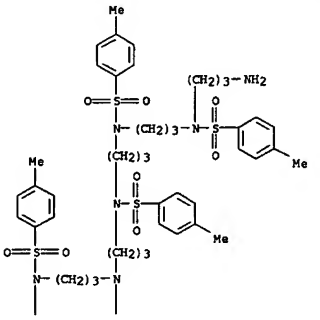

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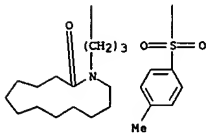
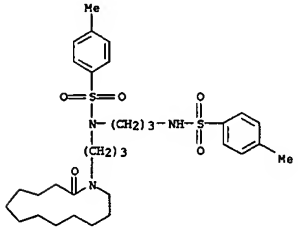
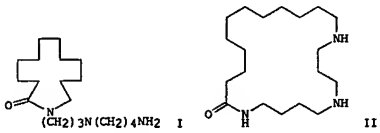


IT **73100-41-1P 73100-42-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 73100-41-1 CAPLUS
CN Azacyclotridecan-2-one, 1-[41-phenyl-40-(phenylmethyl)-4,8,12,16,20,24,28,32,36-nonaazahentetracont-1-yl]-, decahydrochloride (9CI) (CA INDEX NAME)

L4 ANSWER 18 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
CN Benzenesulfonamide, 4-methyl-N-[3-[[(4-methylphenyl)sulfonyl]amino]propyl]-N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

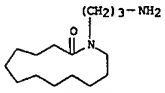


L4 ANSWER 19 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1980:93862 CAPLUS
DOCUMENT NUMBER: 92:93862
TITLE: Transamidation reactions. Part 7. Ring enlargement reactions of N-(2-aminoethyl), N-(4-aminobutyl), N-(6-amino-4-azahexyl), and N-(8-amino-4-azaoctyl) lactams
AUTHOR(S): Stephanou, Euripides; Guggisberg, Armin; Hesse, Manfred
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, CH-8057, Switz.
SOURCE: Helvetica Chimica Acta (1979), 62(6), 1932-43
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



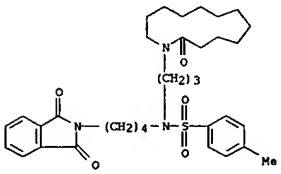
AB Five N-(aminoalkyl) lactams, with 7-, 8-, 9- and 13-membered rings, e.g., I, were prepd. and treated with KNH(CH2)3NH2 in H2N(CH2)3NH2. The caprolactam was stable and did not react, but the others rearranged with ring enlargement; e.g., I rearranged rapidly to a 17-membered ring and, after a longer period, to the 22-membered ring II and H2N(CH2)3NHCO(CH2)11NH(CH2)3NH(CH2)4NH2. The results show that the 7-membered lactam ring was more stable than the 10-membered ring to which it did not rearrange, but the 8-membered lactam ring was less stable than the 11-membered ring to which it did rearrange.

IT **64414-61-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with benzaldehyde followed by redn.)
RN 64414-61-5 CAPLUS
CN Azacyclotridecan-2-one, 1-(3-aminopropyl)- (9CI) (CA INDEX NAME)

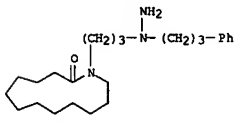


IT **72636-91-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

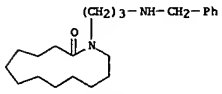
L4 ANSWER 19 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



IT **72636-86-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and hydrogenolysis of)
RN 72636-86-3 CAPLUS
CN Azacyclotridecan-2-one, 1-[3-[1-(3-phenylpropyl)hydrazino]propyl]- (9CI) (CA INDEX NAME)

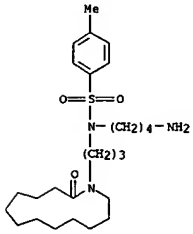


IT **72636-84-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and phthalimido ethylation of)
RN 72636-84-1 CAPLUS
CN Azacyclotridecan-2-one, 1-[3-[(phenylmethyl)amino]propyl]- (9CI) (CA INDEX NAME)

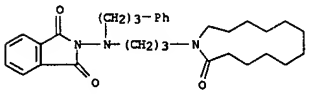


IT **72636-88-5P 72636-92-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and ring enlargement reaction of)
RN 72636-88-5 CAPLUS
CN Azacyclotridecan-2-one, 1-[3-[(2-aminoethyl)amino]propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 19 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
(Reactant or reagent)
(prepn. and detosylation of)
RN 72636-91-0 CAPLUS
CN Benzenesulfonamide, N-(4-aminobutyl)-4-methyl-N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

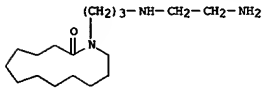


IT **72636-85-2P 72636-90-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and hydrazinolysis of)
RN 72636-85-2 CAPLUS
CN 1H-Isoindole-1,3(2H)-dione, 2-[[3-(2-oxoazacyclotridec-1-yl)propyl](3-phenylpropyl)amino]- (9CI) (CA INDEX NAME)

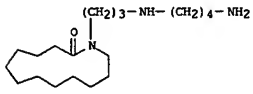


RN 72636-90-9 CAPLUS
CN Benzenesulfonamide, N-[4-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)butyl]-4-methyl-N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

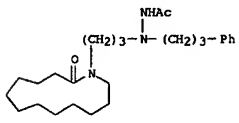
L4 ANSWER 19 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



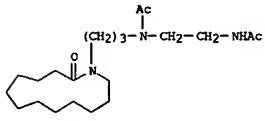
RN 72636-92-1 CAPLUS
CN Azacyclotridecan-2-one, 1-[3-[(4-aminobutyl)amino]propyl]- (9CI) (CA INDEX NAME)



IT **72636-87-4P 72636-89-6P 72636-93-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 72636-87-4 CAPLUS
CN Acetic acid, 2-[3-(2-oxoazacyclotridec-1-yl)propyl]-2-(3-phenylpropyl)hydrazide (9CI) (CA INDEX NAME)

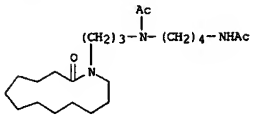


RN 72636-89-6 CAPLUS
CN Acetamide, N-[2-(acetylamino)ethyl]-N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

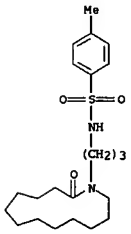


RN 72636-93-2 CAPLUS
CN Acetamide, N-[4-(acetylamino)butyl]-N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

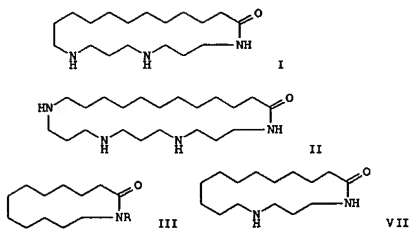
L4 ANSWER 19 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



IT **67370-84-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with (bromobutyl)phthalamide)
RN 67370-84-7 CAPLUS
CN Benzenesulfonamide, 4-methyl-N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



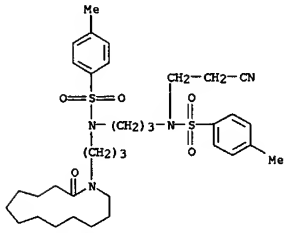
L4 ANSWER 20 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1978:509418 CAPLUS
DOCUMENT NUMBER: 89:109418
TITLE: The Zip reaction: a new ring expansion reaction. Synthesis of 17-, 21- and 25-membered polyaminolactams
AUTHOR(S): Kramer, Urs; Guggisberg, Armin; Hesse, Manfred; Schmid, Hans
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, Switz.
SOURCE: Helvetica Chimica Acta (1978), 61(4), 1342-52
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



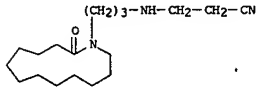
AB The 21- and 25-membered aminolactams I and II were prepd. by introducing the ring enlargement unit (aminopropyl group) into III (R = H), followed by conversion into the heterocyclic lactam by strong base. N-alkylation of III (R = H) with H2C:CHCN, followed by hydrogenation gave III [R = (CH2)3NH2] (IV), and repetition of this process once and twice gave III [R = (CH2)3NH(CH2)3NH2] (V) and III [R = (CH2)3NH(CH2)3NH(CH2)3NH2] (VI). Treatment of IV, V, and VI with base (zip reaction) gave the lactams VII, I and II, resp. I was also obtained stepwise by aminopropylation and ring enlargement of VII.

IT **67171-90-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and deblocking of)
RN 67171-90-8 CAPLUS
CN Benzenesulfonamide, N-(2-cyanoethyl)-4-methyl-N-[3-[[(4-methylphenyl)sulfonyl][3-(2-oxoazacyclotridec-1-yl)propyl]amino]propyl]- (9CI) (CA INDEX NAME)

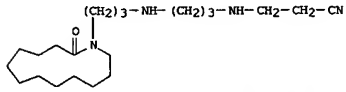
L4 ANSWER 20 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



IT **67171-82-8P 67171-91-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and redn. of)
RN 67171-82-8 CAPLUS
CN Propanenitrile, 3-[[3-(2-oxoazacyclotridec-1-yl)propyl]amino]- (9CI) (CA INDEX NAME)

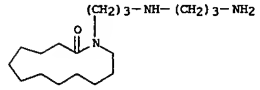


RN 67171-91-9 CAPLUS
CN Propanenitrile, 3-[[3-[[3-(2-oxoazacyclotridec-1-yl)propyl]amino]propyl]amino]- (9CI) (CA INDEX NAME)

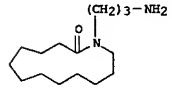


IT **64414-60-4P 64414-61-5P 67473-75-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and ring expansion of)
RN 64414-60-4 CAPLUS
CN Azacyclotridecan-2-one, 1-[3-[(3-aminopropyl)amino]propyl]- (9CI) (CA INDEX NAME)

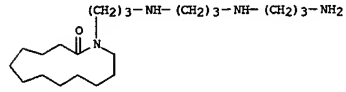
L4 ANSWER 20 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



RN 64414-61-5 CAPLUS
CN Azacyclotridecan-2-one, 1-(3-aminopropyl)- (9CI) (CA INDEX NAME)

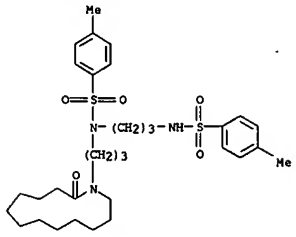


RN 67473-75-0 CAPLUS
CN Azacyclotridecan-2-one, 1-[3-[[3-[(3-aminopropyl)amino]propyl]amino]propyl]- (9CI) (CA INDEX NAME)

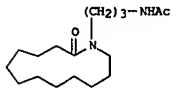


IT **65545-59-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and N-alkylation of, by acrylonitrile)
RN 65545-59-7 CAPLUS
CN Benzenesulfonamide, 4-methyl-N-[3-[[(4-methylphenyl)sulfonyl]amino]propyl]-N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

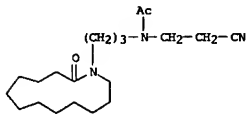
L4 ANSWER 20 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



IT **67171-81-7P 67171-83-9P 67171-92-0P**
67473-76-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 67171-81-7 CAPLUS
CN Acetamide, N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

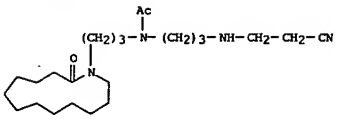


RN 67171-83-9 CAPLUS
CN Acetamide, N-(2-cyanoethyl)-N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

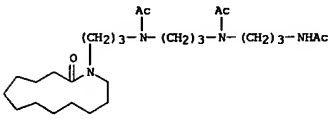


RN 67171-92-0 CAPLUS
CN Acetamide, N-[3-[(2-cyanoethyl)amino]propyl]-N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 20 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

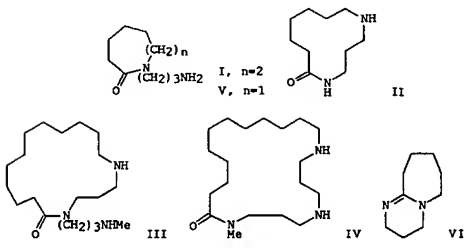


RN 67473-76-1 CAPLUS
CN Acetamide, N-[3-(acetylamino)propyl]-N-[3-[acetyl[3-(2-oxoazacyclotridec-1-yl)propyl]amino]propyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 21 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN

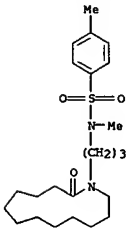
ACCESSION NUMBER: 1978:509412 CAPLUS
DOCUMENT NUMBER: 89:109412
TITLE: Transamidation reactions of cyclic amino amides
AUTHOR(S): Guggisberg, Armin; Kramer, Urs; Heidelberger, Christian; Charubala, Ramamurty; Stephanou, Euripides; Hesse, Manfred; Schmid, Hans
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, Switz.
SOURCE: Helvetica Chimica Acta (1978), 61(3), 1050-63
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



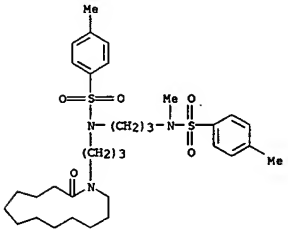
AB Lactams which are substituted at the N atom by a 3-aminopropyl residue were transformed under base catalysis to a cyclic amide enlarged by 4 ring atoms. The formed rings must have a min. of 12 members. Thus, the lactam I was transamidated in 96% yield to give the 12-membered ring II in the presence of H2NCH2CH2CONH2.K in H2N(CH2)3NH2. Large ring lactams which are substituted at the N by a 3-(alkylamino)propyl group lead under base catalysis to an equil. mixt., e.g. the 17-membered lactam III was in equil. with the 21-membered amino amide IV. Transamidation of the lactam V didn't give the expected amino amide, but gave the water elimination product VI.

IT **67370-85-8P 67370-88-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and detosylation of)
RN 67370-85-8 CAPLUS
CN Benzenesulfonamide, N,4-dimethyl-N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 21 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

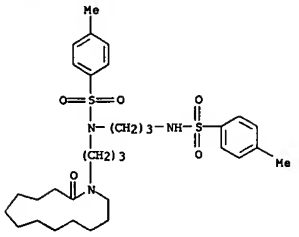


RN 67370-88-1 CAPLUS
CN Benzenesulfonamide, N,4-dimethyl-N-[3-[[(4-methylphenyl)sulfonyl][3-(2-oxoazacyclotridec-1-yl)propyl]amino]propyl]- (9CI) (CA INDEX NAME)

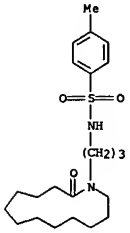


IT **65545-59-7P 67370-84-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and methylation of)
RN 65545-59-7 CAPLUS
CN Benzenesulfonamide, 4-methyl-N-[3-[[(4-methylphenyl)sulfonyl]amino]propyl]-N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 21 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

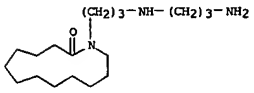


RN 67370-84-7 CAPLUS
CN Benzenesulfonamide, 4-methyl-N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



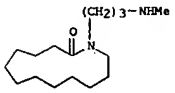
IT **67370-86-9P 67370-89-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and transamidation of)
RN 67370-86-9 CAPLUS
CN Azacyclotridecan-2-one, 1-[3-(methylamino)propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 21 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

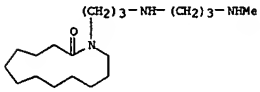


●x HCl

L4 ANSWER 21 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

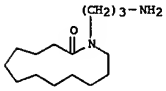


RN 67370-89-2 CAPLUS
CN Azacyclotridecan-2-one, 1-[3-[[3-(methylamino)propyl]amino]propyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

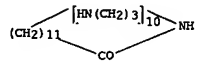
IT **64414-61-5 67370-92-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with toluenesulfonyl chloride)
RN 64414-61-5 CAPLUS
CN Azacyclotridecan-2-one, 1-(3-aminopropyl)- (9CI) (CA INDEX NAME)



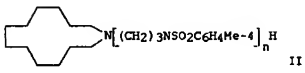
RN 67370-92-7 CAPLUS
CN Azacyclotridecan-2-one, 1-[3-[(3-aminopropyl)amino]propyl]-, hydrochloride (9CI) (CA INDEX NAME)

L4 ANSWER 22 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1978:136588 CAPLUS
DOCUMENT NUMBER: 88:136588
TITLE: Transamidation reactions. 5. Application of the "zip" reaction to the synthesis of a 53-membered polyaminolactam
AUTHOR(S): Kramer, Urs; Guggisberg, Armin; Hesse, Manfred; Schmid, Hans
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, Switz.
SOURCE: Angewandte Chemie (1978), 90(3), 210-11
CODEN: ANCEAD; ISSN: 0044-8249
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



I

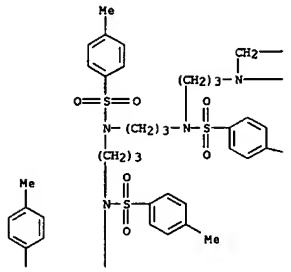


II

AB The macrocycle I was prepd. from N-(3-brompropyl)phthalimide and tosylhydrazine via II (n = 2, 6, 10).
IT **65605-33-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and deblocking of)
RN 65605-33-6 CAPLUS
CN Benzenesulfonamide, 4-methyl-N-[4,8,12,16-tetrakis[(4-methylphenyl)sulfonyl]-19-(2-oxoazacyclotridec-1-yl)-4,8,12,16-tetraazanonadec-1-yl]-N-[4,8,12,16-tetrakis[(4-methylphenyl)sulfonyl]-21-phenyl-20-(phenylmethyl)-4,8,12,16,20-pentaazaheneicos-1-yl]- (9CI) (CA INDEX NAME)

L4 ANSWER 22 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 1-A



PAGE 1-B

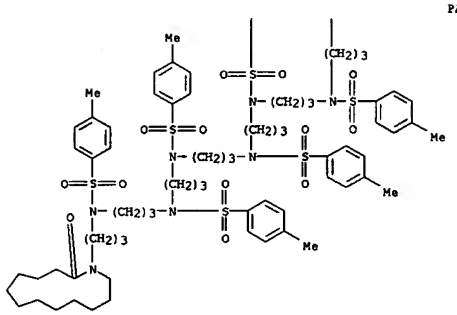
— Ph

— CH_2 — Ph

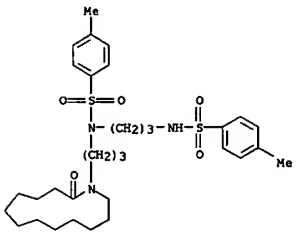
— Me

L4 ANSWER 22 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

PAGE 2-A



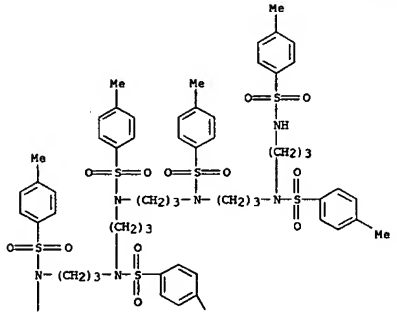
IT **65545-59-7P 65605-32-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with phthalimidotricosyltriazapentadecane)
RN 65545-59-7 CAPLUS
CN Benzenesulfonamide, 4-methyl-N-[3-[[(4-methylphenyl)sulfonyl]amino]propyl]-N-[3-(2-oxoazacyclotridec-1-yl)propyl]- (9CI) (CA INDEX NAME)



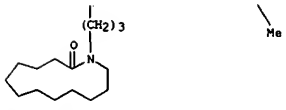
RN 65605-32-5 CAPLUS
CN Benzenesulfonamide, 4-methyl-N-[3-[[(4-methylphenyl)sulfonyl][3-[[(4-methylphenyl)sulfonyl]amino]propyl]amino]propyl]-N-[3-[[(4-

L4 ANSWER 22 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
methylphenyl)sulfonyl][3-[[(4-methylphenyl)sulfonyl][3-[[(4-methylphenyl)sulfonyl][3-[(2-oxoazacyclotridec-1-yl)amino]propyl]amino]propyl]amino]propyl]amino]propyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



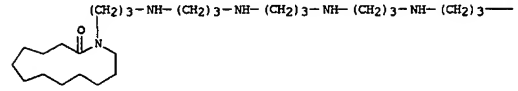
PAGE 2-A



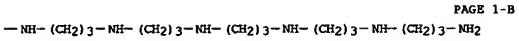
IT **65605-34-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and rearrangement of)
RN 65605-34-7 CAPLUS
CN Azacyclotridecan-2-one, 1-(39-amino-4,8,12,16,20,24,28,32,36-nonaazanonatriacont-1-yl)- (9CI) (CA INDEX NAME)

L4 ANSWER 22 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

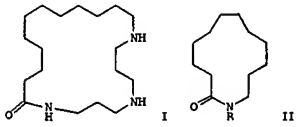
PAGE 1-A



PAGE 1-B



L4 ANSWER 23 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1978:37595 CAPLUS
DOCUMENT NUMBER: 88:37595
TITLE: Transamidation reactions. 2. The "zip" reaction: a new method for ring enlargement; synthesis of 17- and 21-membered polyaminolactams
AUTHOR(S): Kramer, Urs; Guggisberg, Armin; Hesse, Manfred; Schmid, Hans
CORPORATE SOURCE: Org.-Chem. Inst., Univ. Zurich, Zurich, Switz.
SOURCE: Angewandte Chemie (1977), 89(12), 899-900
CODEN: ANCEAD; ISSN: 0044-8249
DOCUMENT TYPE: Journal
LANGUAGE: German
GI

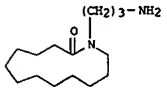


I II

AB Triazacycloheneicosanone I was prepd. by treating the azacyclotridecanone II (R = Na) with CH2:CHCN and hydrogenation of II (R = CH2CH2CN) to give 82% II [R = (CH2)3NH2]. Repetition of the sequence gave 78% II [R = (CH2)3NH(CH2)3NH2], which on treatment with KNH(CH2)3NH2 gave 90% I.

IT **64414-61-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with acrylonitrile)

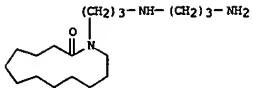
RN 64414-61-5 CAPLUS
CN Azacyclotridecan-2-one, 1-(3-aminopropyl)- (9CI) (CA INDEX NAME)



IT **64414-60-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and rearrangement of, with aminopropylamide)

RN 64414-60-4 CAPLUS
CN Azacyclotridecan-2-one, 1-[3-[(3-aminopropyl)amino]propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 23 OF 23 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	119.50	267.86

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-16.28	-16.28

STN INTERNATIONAL LOGOFF AT 16:59:50 ON 06 AUG 2003

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4	1739		USPAT	2003/08/06 17:42
5	81	(514/183, 540/450, 540/451) and angiogenesis$	USPAT	2003/08/06 17:43